



STIC Search Report

EIC 1700

STIC Database Tracking Number: 171713

**TO: Ben Sackey
Location: REM 5B31
Art Unit : 1626
November 18, 2005**

Case Serial Number: 10/695015

**From: Kathleen Fuller
Location: EIC 1700
REMSSEN 4B28
Phone: 571/272-2505
Kathleen.Fuller@uspto.gov**

Search Notes

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Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: BEN SACKER Examiner #: 73489 Date: 11/15/05
Art Unit: 1628 Phone Number: 2-0704 Serial Number: 10/695,015
Location (Bldg/Room#): RM 5B37 (Mailbox #): _____ Results Format Preferred (circle): PAPER DISK

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Hydrocyanation of pentenenitriles and/or 2-methyl-3-butenitrile using process obtained by chlorination of titanium-vacInventors (please provide full names): Too et al

Earliest Priority Date: _____

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

A process for the hydrocyanation of at least one substrate selected from 2-pentenitrile, 3-pentenitrile, 4-pentenitrile and 2-methyl-3-butenitrile with hydrogen cyanide in the presence of zero-valent nickel catalyst

SCIENTIFIC REFERENCE BR
Sci & Tech Inf - Cntr

NOV 16 REC'D

Pat. & T.M. Office

STAFF USE ONLY

Searcher: Fuller Type of Search: _____
NA Sequence (#) _____
Searcher Phone: _____
SA Sequence (#) _____
Searcher Location: 4 Structure (#) _____
Bibliographic _____
Date Searcher Picked Up: _____

Vendors and cost where applicable

☒ STN _____ Dialog _____
Questel/Orbit _____ Lexis/Nexis _____
Westlaw _____ WWW/Internet _____
In-house sequence systems _____

Date of Issue: 11/18/05 _____
Searcher Fee & Ref. Fee: 40 _____
Online Time: 25 _____
Fulltext _____
Other _____

Commercial _____ Oligomer _____ Score/Length _____
Interference _____ SPDI _____ Encoder/Translator _____
Other (specify) _____

=> FILE REG

FILE 'REGISTRY' ENTERED AT 15:56:25 ON 18 NOV 2005

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 17 NOV 2005 HIGHEST RN 868355-11-7

DICTIONARY FILE UPDATES: 17 NOV 2005 HIGHEST RN 868355-11-7

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

=> FILE HCAPL

FILE 'HCAPLUS' ENTERED AT 15:56:29 ON 18 NOV 2005

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FILE COVERS 1907 - 18 Nov 2005 VOL 143 ISS 22

FILE LAST UPDATED: 17 Nov 2005 (20051117/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> D QUE

L47 3 SEA FILE=REGISTRY ABB=ON 592-51-8 OR 4636-87-4 OR 13284-42-9
OR 16529-56-9
L48 4 SEA FILE=REGISTRY ABB=ON L47 OR 4635-87-4 — *nitriles in claims*
L49 1 SEA FILE=REGISTRY ABB=ON 74-90-8 — *HCN*
L50 558 SEA FILE=HCAPLUS ABB=ON L48
L51 301 SEA FILE=HCAPLUS ABB=ON L50 (L) RACT/RL
L52 16050 SEA FILE=HCAPLUS ABB=ON L49
L53 2455 SEA FILE=HCAPLUS ABB=ON L52 (L) RACT/RL
L54 45 SEA FILE=HCAPLUS ABB=ON L51 AND L53
L55 40 SEA FILE=HCAPLUS ABB=ON L54 AND CAT/RL
L57 16 SEA FILE=HCAPLUS ABB=ON HYDROCYAN? (4A) (SUBSTRATE? OR SURFACE?)

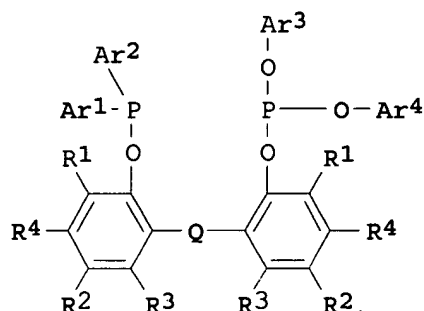
L58 2 SEA FILE=HCAPLUS ABB=ON L55 AND L57
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L60 2 SEA FILE=HCAPLUS ABB=ON L50 AND L52 AND L57
L62 58 SEA FILE=HCAPLUS ABB=ON L50 AND L52 AND HYDROCYANAT?
L63 40 SEA FILE=HCAPLUS ABB=ON L51 AND L62
L64 40 SEA FILE=HCAPLUS ABB=ON L63 AND (CAT/RL OR CATALY?)
L65 2 SEA FILE=HCAPLUS ABB=ON L64 AND (SUBSTRATE? OR SURFACE?)
L66 2 SEA FILE=HCAPLUS ABB=ON L50 AND L57
L67 16 SEA FILE=HCAPLUS ABB=ON L64 AND PROMOT?
L68 17 SEA FILE=HCAPLUS ABB=ON (L58 OR L59 OR L60) OR (L65 OR L66 OR
— L67)

=> D L68 BIB ABS IND HITSTR 1-17

L68 ANSWER 1 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:409533 HCAPLUS
DN 142:430424
TI Design and preparation of sterically hindered chelate phosphinite-
phosphite ligands for nickel-catalyzed preparation of nitriles
and dinitriles by hydrocyanation of unsaturated compounds
IN Bartsch, Michael; Baumann, Robert; Haderlein, Gerd; Flores, Miguel Angel;
Jungkamp, Tim; Luyken, Hermann; Scheidel, Jens; Siegel, Wolfgang
PA BASF Aktiengesellschaft, Germany
SO PCT Int. Appl., 33 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2005042547	A1	20050512	WO 2004-EP12176	20041028
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
	RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	DE 10350999	A1	20050602	DE 2003-10350999	20031030

PRAI DE 2003-10350999 A 20031030
 OS MARPAT 142:430424
 GI



I

AB The 2,2'-biphenol, 2,2'-methylenebis(phenol) and 2,2'-binaphthol-bridged phosphinite-phosphite ligands, preferably of the type I (Ar1, Ar2 = Ph, fluoro- and trifluoromethyl-substituted Ph, preferably 3-FC6H4, 3,5-F2C6H3, 3-(CF3)C6H4, 3,5-(CF3)2C6H3; Ar3 = Ar4 = 2-MeC6H4; Q = (CH2)n, where n = 0, 1; R1, R2, R4 = H, C1-8 (un)saturated hydrocarbyl; R3 = H, Me, Et; or R2-R3 = (CH)4, same R1, R2, R4) are designed for nickel(0)-catalyzed hydrocyanation of butadiene to give 3-pentenitrile and adiponitrile in the presence of Lewis acid promoters, such as metal chlorides and triflates. In an example, ligand of the type I (2, Ar1 = Ar2 = Ph, Ar3 = Ar4 = 2-MeC6H4, R1 = R2 = Me, R3 = R4 = H) was prepared by reaction of 3,3',5,5'-tetramethyl-2,2'-biphenol with Ph2PCl and (2-MeC6H4O)2PCl in toluene at -15°.

Hydrocyanation of 1,3-butadiene by HCN catalyzed by Ni(cod)2/2 (1:3 mol. ratio; C4H6/HCN = 1.6:1; 0.135 mol % of the catalyst) gave a 1.5:1 mixture of 2-methyl-3-butenitrile and 3-pentenitrile; the ratio was enhanced to 1:4.6 upon isomerization during 1 h at 115°. In another example, 3-pentenitrile was hydrocyanated to adiponitrile with the same catalyst at 25° for 88 min in the presence of ZnCl2 with regioselectivity of 91.3%. In comparison examples, use of o- and m-tolyl phosphite nickel(0) complex gave only 79.6% selectivity on adiponitrile.

IC ICM C07F009-50

ICS C07F009-12; B01J031-24

CC 29-7 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 23

ST phosphorus ligand bidentate diene unsatd nitrile **hydrocyanation catalyst**; nitrile dinitrile improved prepn process phosphinite phosphite ligand **catalyst**; nickel **catalyzed hydrocyanation** phosphinite phosphite bidentate sterically hindered ligand; butadiene pentenenitrile **hydrocyanation** improved process nickel phosphinite phosphite **catalyst**; isomerization unsatd nitrile **hydrocyanation** nickel phosphinite phosphite **catalyst**; adiponitrile improved prepn regioselective **hydrocyanation** process nickel **catalyst**; addn reaction diene unsatd nitrile **hydrocyanation** adiponitrile improved prepn

IT Ligands

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

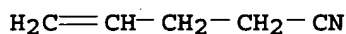
(bidentate, phosphinites, phosphites; design and preparation of sterically hindered phosphinite-phosphite bidentate chelate ligands for nickel-catalyzed hydrocyanation of dienes and unsatd.

- nitriles improved process)
- IT Addition reaction
Hydrocyanation
Hydrocyanation catalysts
Regiochemistry
(design and preparation of sterically hindered phosphinite-phosphite bidentate chelate ligands for nickel-catalyzed hydrocyanation of dienes and unsatd. nitriles improved process)
- IT Chelates
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(design and preparation of sterically hindered phosphinite-phosphite bidentate chelate ligands for nickel-catalyzed hydrocyanation of dienes and unsatd. nitriles improved process)
- IT Alkadienes
RL: RCT (Reactant); RACT (Reactant or reagent)
(design and preparation of sterically hindered phosphinite-phosphite bidentate chelate ligands for nickel-catalyzed hydrocyanation of dienes and unsatd. nitriles improved process)
- IT Steric hindrance
(design and preparation of sterically hindered phosphinite-phosphite bidentate ligands for nickel-catalyzed hydrocyanation of dienes and unsatd. nitriles improved process)
- IT Nitriles, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(dinitriles; design and preparation of sterically hindered phosphinite-phosphite bidentate chelate ligands for nickel-catalyzed hydrocyanation of dienes and unsatd. nitriles improved process)
- IT Isomerization
(double bond migration in unsatd. nitriles catalyzed by sterically hindered phosphinite-phosphite bidentate nickel complexes in improved process for regioselective hydrocyanation of butadiene)
- IT Phosphorus acids
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(esters, phosphinites; design and preparation of sterically hindered phosphinite-phosphite bidentate chelate ligands for nickel-catalyzed hydrocyanation of dienes and unsatd. nitriles improved process)
- IT Phosphites
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(phosphinites, phosphites; design and preparation of sterically hindered phosphinite-phosphite bidentate chelate ligands for nickel-catalyzed hydrocyanation of dienes and unsatd. nitriles improved process)
- IT Nitriles, preparation
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(unsatd.; isomerization and hydrocyanation of unsatd. nitriles catalyzed by nickel phosphinite-phosphite bidentate chelate complexes in adiponitrile improved preparation process)
- IT 26567-10-2 110932-47-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(esterification; regioselective hydrocyanation of butadiene and unsatd. nitriles catalyzed by phosphinite-phosphite bidentate chelate nickel complexes in improved process for preparation of adiponitrile)

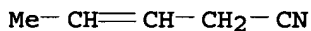
- IT 74-90-8, Hydrocyanic acid, reactions 106-99-0, 1,3-Butadiene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrocyanation; regioselective hydrocyanation of butadiene and unsatd. nitriles catalyzed by phosphinite-phosphite bidentate chelate nickel complexes in improved process for preparation of adiponitrile)
- IT 592-51-8P, 4-Pentenitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(hydrocyanation; regioselective hydrocyanation of butadiene and unsatd. nitriles catalyzed by phosphinite-phosphite bidentate chelate nickel complexes in improved process for preparation of adiponitrile)
- IT 4635-87-4P, 3-Pentenitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(isomerization, hydrocyanation; regioselective hydrocyanation of butadiene and unsatd. nitriles catalyzed by phosphinite-phosphite bidentate chelate nickel complexes in improved process for preparation of adiponitrile)
- IT 16529-56-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(isomerization; regioselective hydrocyanation of butadiene and unsatd. nitriles catalyzed by phosphinite-phosphite bidentate chelate nickel complexes in improved process for preparation of adiponitrile)
- IT 7440-02-0D, Nickel, complexes, phosphinite-phosphite 7646-85-7, Zinc chloride, uses
RL: CAT (Catalyst use); USES (Uses)
(regioselective hydrocyanation of butadiene and unsatd. nitriles catalyzed by phosphinite-phosphite bidentate chelate nickel complexes in improved process for preparation of adiponitrile)
- IT 851024-54-9P 851024-55-0P 851024-56-1P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(regioselective hydrocyanation of butadiene and unsatd. nitriles catalyzed by phosphinite-phosphite bidentate chelate nickel complexes in improved process for preparation of adiponitrile)
- IT 111-69-3P, Adiponitrile
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(regioselective hydrocyanation of butadiene and unsatd. nitriles catalyzed by phosphinite-phosphite bidentate chelate nickel complexes in improved process for preparation of adiponitrile)
- IT 1079-66-9, Chlorodiphenylphosphine 1295-35-8 22277-50-5 33104-14-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective hydrocyanation of butadiene and unsatd. nitriles catalyzed by phosphinite-phosphite bidentate chelate nickel complexes in improved process for preparation of adiponitrile)
- IT 74-90-8, Hydrocyanic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrocyanation; regioselective hydrocyanation of butadiene and unsatd. nitriles catalyzed by phosphinite-phosphite bidentate chelate nickel complexes in improved process for preparation of adiponitrile)
- RN 74-90-8 HCAPLUS
CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)

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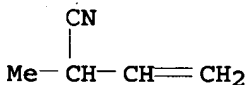
IT 592-51-8P, 4-Pentenitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(hydrocyanation; regioselective hydrocyanation of
butadiene and unsatd. nitriles catalyzed by
phosphinite-phosphite bidentate chelate nickel complexes in improved
process for preparation of adiponitrile)
RN 592-51-8 HCAPLUS
CN 4-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 4635-87-4P, 3-Pentenitrile
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(isomerization, hydrocyanation; regioselective
hydrocyanation of butadiene and unsatd. nitriles
catalyzed by phosphinite-phosphite bidentate chelate nickel
complexes in improved process for preparation of adiponitrile)
RN 4635-87-4 HCAPLUS
CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 16529-56-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
RACT (Reactant or reagent)
(isomerization; regioselective hydrocyanation of butadiene
and unsatd. nitriles catalyzed by phosphinite-phosphite
bidentate chelate nickel complexes in improved process for preparation of
adiponitrile)
RN 16529-56-9 HCAPLUS
CN 3-Butenenitrile, 2-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L68 ANSWER 2 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2005:371050 HCAPLUS
DN 142:413302
TI Catalytic hydrocyanation of pentenenitriles and/or
2-methyl-3-butenitrile using promoters obtained from the
chlorination of titanium-rich ores
IN Foo, Thomas; Lenges, Christian Peter

applicants

PA USA
 SO U.S. Pat. Appl. Publ., 10 pp.
 CODEN: USXXCO
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2005090681	A1	20050428	US 2003-695015	20031028
	EP 1528054	A1	20050504	EP 2004-256674	20041028
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
PRAI	US 2003-695015	A	20031028		
AB	A process for hydrocyanating a substrate selected from 2-, 3-, or 4-pentenitrile and/or 2-methyl-3-butenitrile, or their mixts., comprises contacting the substrate with HCN in the presence of a zero-valent nickel catalyst and a promoter that is obtained as a byproduct of titanium ore chlorination.				
IC	ICM C07C253-10				
INCL	558348000				
CC	45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes) Section cross-reference(s): 48, 67				
ST	pentenenitrile catalytic hydrocyanation ; methylbutenenitrile catalytic hydrocyanation				
IT	Hydrocyanation Hydrocyanation catalysts (catalytic hydrocyanation of pentenenitriles and/or 2-methyl-3-butenitrile using promoters obtained from the chlorination of titanium-rich ores)				
IT	Chlorination (of Ti-rich ore in the preparation of hydrocyanation catalysts)				
IT	Nitriles, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (unsatd.; catalytic hydrocyanation of pentenenitriles and/or 2-methyl-3-butenitrile using promoters obtained from the chlorination of titanium-rich ores)				
IT	7440-02-0, Nickel, uses 7758-94-3, Ferrous chloride 7773-01-5, Manganese dichloride RL: CAT (Catalyst use) ; USES (Uses) (catalytic hydrocyanation of pentenenitriles and/or 2-methyl-3-butenitrile using promoters obtained from the chlorination of titanium-rich ores)				
IT	7550-45-0P, Titanium tetrachloride, preparation RL: CAT (Catalyst use) ; SPN (Synthetic preparation) ; PREP (Preparation) ; USES (Uses) (catalytic hydrocyanation of pentenenitriles and/or 2-methyl-3-butenitrile using promoters obtained from the chlorination of titanium-rich ores)				
IT	74-90-8, Hydrogen cyanide, reactions 592-51-8, 4-Pentenitrile 4635-87-4, 3-Pentenitrile 13284-42-9, 2-Pentenitrile 16529-56-9, 2-Methyl-3-butenitrile RL: RCT (Reactant); RACT (Reactant or reagent) (catalytic hydrocyanation of pentenenitriles and/or 2-methyl-3-butenitrile using promoters obtained from the chlorination of titanium-rich ores)				
IT	74-90-8, Hydrogen cyanide, reactions 592-51-8, 4-Pentenitrile 4635-87-4, 3-Pentenitrile 13284-42-9, 2-Pentenitrile 16529-56-9, 2-Methyl-3-butenitrile RL: RCT (Reactant); RACT (Reactant or reagent)				

(catalytic hydrocyanation of pentenenitriles and/or
2-methyl-3-butenitrile using promoters obtained from the
chlorination of titanium-rich ores)

RN 74-90-8 HCAPLUS
CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)



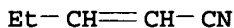
RN 592-51-8 HCAPLUS
CN 4-Pentenenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



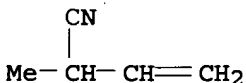
RN 4635-87-4 HCAPLUS
CN 3-Pentenenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 13284-42-9 HCAPLUS
CN 2-Pentenenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



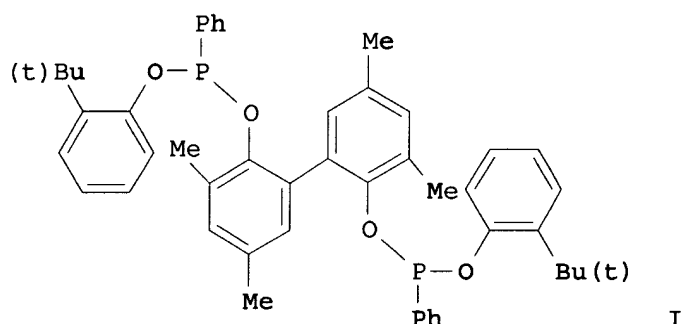
RN 16529-56-9 HCAPLUS
CN 3-Butenenitrile, 2-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L68 ANSWER 3 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:841730 HCAPLUS
DN 141:351754
TI Nickel complex **catalytic** system for **hydrocyanation** of
olefins
IN Bartsch, Michael; Baumann, Robert; Haderlein, Gerd; Flores, Miguel;
Jungkamp, Tim; Luyken, Hermann; Scheidel, Jens; Siegel, Wolfgang; Molnar,
Ferenc
PA BASF AG, Germany
SO Ger. Offen., 19 pp.
CODEN: GWXXBX
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10314761	A1	20041014	DE 2003-10314761	20030331

WO 2004087314 A1 20041014 WO 2004-EP3103 20040324
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
TD, TG
PRAI DE 2003-10314761 A 20030331
OS MARPAT 141:351754
GI



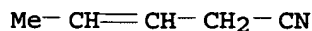
- AB A **catalytic system useful for hydrocyanation** of unsatd. nitriles in the manufacture of adiponitrile comprises (A) Ni(0), (B) trivalent P-compound as ligand for complexing Ni(0), (C) a Lewis acid, and (D) a compound of the formula MR_n (M = Al, Ti; R = alkoxy, alkyl; with a proviso; n = valence of M). For example, stirring a mixture of 1 equiv NTP [Ni(0)-tris(m,p-tolyl) phosphite complex containing 2.35% Ni(0), 19% 3-pentenitrile (3-PN) and 78.65% m,p-tolyl phosphite] with 1000 equiv 3-PN and 2 equiv ligand I for 1 h at 25°, heating the mixture to 60°, adding 1 equiv AlEt₃ and 1 equiv ZnCl₂, stirring for 5 min and introducing 303 equiv HCN(g)/h·Ni under Ar gave, after 140 min, 64% adiponitrile (ADP) with 95.5% selectivity for ADP, vs. 35.8% yield and 94.8% selectivity for a similar run without AlEt₃.
- IC ICM B01J031-18
ICS B01J031-12; B01J031-24; C07B043-08; C07C253-10; C07C255-04
- CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 67
- ST nickel complex **catalyst** olefin **hydrocyanation**;
pentenenitrile **hydrocyanation** nickel complex **catalyst**;
Lewis acid synergistic **promoter hydrocyanation**;
adiponitrile manuf nickel complex **hydrocyanation catalyst**
- IT Lewis acids
RL: CAT (Catalyst use); USES (Uses)
(catalyst system components; nickel complex **catalytic system for hydrocyanation** of olefins)
- IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(nickel complex **catalytic system for hydrocyanation**)

of)

- IT **Hydrocyanation catalysts**
(nickel complex catalytic system for hydrocyanation of olefins)
- IT 97-93-8, Triethylaluminum, uses 620-38-2, Tris(m-tolyl) phosphite 620-42-8, p-Tolyl phosphite 3453-79-0, Tri(isobutoxy)aluminum 5593-70-4, Tetraabutoxytitanium 7646-85-7, Zinc chloride, uses 7758-94-3, Ferrous chloride
RL: **CAT (Catalyst use); USES (Uses)**
(catalyst system component; nickel complex catalytic system for hydrocyanation of olefins)
- IT 220472-84-4 509083-87-8 512172-95-1 528597-72-0 774242-20-5 774242-21-6
RL: **CAT (Catalyst use); USES (Uses)**
(ligand; nickel complex catalytic system for hydrocyanation of olefins)
- IT 1295-35-8, Biscyclooctadienenickel 7440-02-0, Nickel, uses
RL: **CAT (Catalyst use); USES (Uses)**
(nickel complex catalytic system for hydrocyanation of olefins)
- IT 111-69-3P, Adiponitrile
RL: IMF (Industrial manufacture); PREP (Preparation)
(nickel complex catalytic system for hydrocyanation of olefins)
- IT 592-51-8, 4-Pentenitrile 4635-87-4, 3-Pentenitrile
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(nickel complex catalytic system for hydrocyanation of olefins)
- IT 74-90-8, Hydrocyanic acid, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(nickel complex catalytic system for hydrocyanation of olefins with)
- IT 592-51-8, 4-Pentenitrile 4635-87-4, 3-Pentenitrile
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(nickel complex catalytic system for hydrocyanation of olefins)
- RN 592-51-8 HCAPLUS
CN 4-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



- RN 4635-87-4 HCAPLUS
CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



- IT 74-90-8, Hydrocyanic acid, reactions
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(nickel complex catalytic system for hydrocyanation of olefins with)
- RN 74-90-8 HCAPLUS
CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)

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L68 ANSWER 4 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:737717 HCAPLUS
DN 139:262467
TI Phosphonite ligands and their use in **hydrocyanation**
IN Lenges, Christian P.; Lu, Helen S. M.; Ritter, Joachim C.
PA E. I. Du Pont de Nemours & Co., USA
SO PCT Int. Appl., 25 pp.
CODEN: PIXXD2

DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2003076394	A1	20030918	WO 2003-US7033	20030307
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW			
	RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
	US 2003195371	A1	20031016	US 2002-93655	20020307
	US 6660877	B2	20031209		
	US 2003195372	A1	20031016	US 2003-454074	20030604
	US 6737539	B2	20040518		
	US 2003212288	A1	20031113	US 2003-454024	20030604
	US 6846945	B2	20050125		
PRAI	US 2002-93655	A	20020307		

OS MARPAT 139:262467

AB Disclosed herein are processes for **hydrocyanation** and isomerization of olefins by using at least one multidentate phosphonite ligands, including organometallic phosphonite ligands with a Group VIII metal or Group VIII metal compound, and optionally, a Lewis acid **promoter**. Thus, trans-3-pentenitrile was reacted in the presence of bis(1,5-cyclooctadiene) nickel, phosphonite bidentate ligand, and zinc dichloride to give an adiponitrile.

IC ICM C07C253-00

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

ST organometallic multidentate phosphonite ligand **hydrocyanation catalyst** isomerization olefin

IT **Hydrocyanation catalysts**

Isomerization **catalysts**

(phosphonite ligands and their use in **hydrocyanation**)

IT **Hydrocyanation catalysts**

(stereoselective; phosphonite ligands and their use in **hydrocyanation**)

IT 1295-35-8, Bis(1,5-cyclooctadiene) nickel 404873-87-6 405164-70-7
405164-72-9 405164-74-1 600121-71-9 600121-72-0 600121-73-1
600121-74-2 600121-75-3 600121-76-4 600121-77-5 600121-78-6
600121-79-7 600710-58-5

RL: **CAT (Catalyst use); USES (Uses)**
 (phosphonite ligands and their use in **hydrocyanation**)

IT 111-69-3P, Adiponitrile **592-51-8P**, 4-Pentenitrile
4635-87-4P, 3-Pentenitrile 16545-78-1P, cis-3-Pentenitrile
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (phosphonite ligands and their use in **hydrocyanation**)

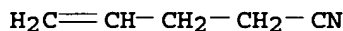
IT **16529-56-9P**, 2-Methyl-3-butenitrile 16529-66-1P,
 trans-3-Pentenitrile
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation);
RACT (Reactant or reagent)
 (phosphonite ligands and their use in **hydrocyanation**)

IT **74-90-8**, Hydrogen cyanide, reactions 106-99-0, 1,3-Butadiene,
 reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (phosphonite ligands and their use in **hydrocyanation**)

IT 7446-70-0, Aluminum trichloride, uses 7646-79-9, Cobalt dichloride, uses
 7646-85-7, Zinc dichloride, uses 12075-68-2, Sesquiethylaluminum
 chloride
 RL: **CAT (Catalyst use); USES (Uses)**
 (promoter; phosphonite ligands and their use in
hydrocyanation)

IT **592-51-8P**, 4-Pentenitrile **4635-87-4P**, 3-Pentenitrile
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (phosphonite ligands and their use in **hydrocyanation**)

RN 592-51-8 HCAPLUS
 CN 4-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

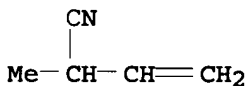


RN 4635-87-4 HCAPLUS
 CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **16529-56-9P**, 2-Methyl-3-butenitrile
 RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation);
RACT (Reactant or reagent)
 (phosphonite ligands and their use in **hydrocyanation**)

RN 16529-56-9 HCAPLUS
 CN 3-Butenenitrile, 2-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT **74-90-8**, Hydrogen cyanide, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (phosphonite ligands and their use in **hydrocyanation**)

RN 74-90-8 HCAPLUS
 CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)

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RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L68 ANSWER 5 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:223752 HCAPLUS

DN 138:254847

TI Process for manufacture of nitrile and dinitrile compounds by reaction of alkenes or unsaturated nitriles with hydrogen cyanide in ionic liquid solvents and application to the production of adiponitrile

IN Basset, Jean Marie; Chauvin, Yves; Galland, Jean Christophe

PA Rhodia Polyamide Intermediates, Fr.

SO Fr. Demande, 22 pp.

CODEN: FRXXBL

DT Patent

LA French

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	FR 2829763	A1	20030321	FR 2001-12040	20010918
	FR 2829763	B1	20041203		
	WO 2003024919	A1	20030327	WO 2002-FR3166	20020917
	W:			AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW	
	RW:			GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG	
	EP 1427695	A1	20040616	EP 2002-779637	20020917
	R:			AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK	
	JP 2005503410	T2	20050203	JP 2003-528767	20020917
	US 2004260112	A1	20041223	US 2004-489838	20040818
PRAI	FR 2001-12040	A	20010918		
	WO 2002-FR3166	W	20020917		

OS CASREACT 138:254847

AB The invention relates to the manufacture of nitriles from unsatd. organic compds. by reaction with HCN. In particular, it relates to manufacture of nitriles used in the synthesis of adiponitrile, an important chemical intermediate for the manufacture of, e.g., hexamethylenediamine and ϵ -caprolactam. The process provides compds. containing ≥ 1 nitrile function by **hydrocyanation**, with HCN, of an organic compound containing ≥ 1 ethylenic unsatn. The reaction takes place in the presence of a **catalytic** system comprising nickel, platinum, or palladium, and an organophosphorus ligand, using an ionic liquid reaction medium. A Lewis acid cocatalyst, functioning as an isomerization **catalyst** for unsatd. nitriles, may also be present. This cocatalyst provides for isomerization of undesired branched unsatd. nitriles to give preferred linear isomers, which undergo **hydrocyanation** to give adiponitrile. The anion of the ionic solvent may also function as a Lewis acid. For instance, the ionic liquid 1-butyl-2,3-dimethylimidazolium

bis(trifluoromethylsulfonyl)amide (I) was prepared in 90% yield from the corresponding imidazolium chloride and lithium amide salts in water at room temperature. I and 2 other imidazolium salts were prepared and tested as solvents and isomerization **catalysts** in a representative **hydrocyanation** reaction mixture. Thus, a mixture of unsatd. C5 nitriles containing 79% 2-methyl-3-butenitrile (II) was subjected to isomerization in a solution of I and heptane in the presence of Ni(COD)₂ (**hydrocyanation catalyst**) and 3-(Ph₂P)C₆H₄SO₃Na (ligand) at 100° for 3 h. The isomerization reaction gave 96% conversion of II, with a 94% yield of the desired linear isomers 3-pentenitrile (III) and 4-pentenitrile, with only 2.4% yield of undesired isomers. In a **hydrocyanation** reaction of III using the same **catalyst** and ligand, I as solvent, Me₂C(OH)CN as the source of HCN, and added ZnCl₂ as an addnl. Lewis acid, desired dinitrile products (including adiponitrile) were obtained in 16.0% yield with 25.9% conversion of III.

IC ICM C07C255-04

CC 23-19 (Aliphatic Compounds)

Section cross-reference(s): 45

ST nitrile unsatd **hydrocyanation** hydrogen cyanide liq ionic solvent; imidazolium ionic liq solvent **hydrocyanation** pentenenitrile; adiponitrile manuf ionic liq solvent imidazolium; isomerization methylbutenenitrile pentenenitrile Lewis acid **catalyst**; nickel palladium platinum phosphine ligand **hydrocyanation catalyst** ionic solvent

IT Isomerization **catalysts**

(Lewis acids; process for manufacture of nitriles by **hydrocyanation** of unsatd. compds. with HCN in ionic liquid solvents)

IT Ligands

RL: CAT (**Catalyst use**); RCT (Reactant); RACT (Reactant or reagent); USES (Uses)

(**hydrocyanation catalyst** component; process for manufacture of nitriles by **hydrocyanation** of unsatd. compds. with HCN in ionic liquid solvents)

IT Nitriles, preparation

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(**hydrocyanation** product; process for manufacture of nitriles by **hydrocyanation** of unsatd. compds. with HCN in ionic liquid solvents)

IT Alkadienes

Alkenes, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(**hydrocyanation substrate**; process for manufacture of nitriles by **hydrocyanation** of unsatd. compds. with HCN in ionic liquid solvents)

IT Lewis acids

RL: CAT (**Catalyst use**); USES (Uses)

(isomerization cocatalyst; process for manufacture of nitriles by **hydrocyanation** of unsatd. compds. with HCN in ionic liquid solvents)

IT **Hydrocyanation catalysts**

(nickel, platinum, or palladium with organophosphorus ligands; process for manufacture of nitriles by **hydrocyanation** of unsatd. compds. with HCN in ionic liquid solvents)

IT Isomerization

(of unsatd. nitriles; process for manufacture of nitriles by **hydrocyanation** of unsatd. compds. with HCN in ionic liquid solvents)

IT Organic compounds, reactions

RL: CAT (**Catalyst use**); RCT (Reactant); RACT (Reactant or

- reagent); USES (Uses)
(phosphorus-containing, **hydrocyanation catalyst**
ligands; process for manufacture of nitriles by **hydrocyanation** of
unsatd. compds. with HCN in ionic liquid solvents)
- IT **Hydrocyanation**
Ionic liquids
(process for manufacture of nitriles by **hydrocyanation** of unsatd.
compds. with HCN in ionic liquid solvents)
- IT Nitriles, preparation
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic
preparation); PREP (Preparation); RACT (Reactant or reagent)
(unsatd., isomerization and **hydrocyanation**; process for
manufacture of nitriles by **hydrocyanation** of unsatd. compds. with
HCN in ionic liquid solvents)
- IT 4403-61-6P, 2-Methyl-2-butenenitrile 13284-42-9P,
2-Pentenitrile
RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation); **RACT**
(Reactant or reagent)
(byproduct; process for manufacture of nitriles by **hydrocyanation**
of unsatd. compds. with HCN in ionic liquid solvents)
- IT 122-52-1, Triethyl phosphite 603-35-0, Triphenylphosphine, reactions
607-01-2, Diphenylethylphosphine 672-66-2, Dimethylphenylphosphine
855-38-9, Tris(p-methoxyphenyl)phosphine 998-40-3, Tributylphosphine
2622-14-2, Tricyclohexylphosphine 4712-55-4, Diphenyl phosphite
7688-25-7, 1,4-Bis(diphenylphosphino)butane 26834-21-9,
Tritolylphosphine 34684-16-7, Dimethyl-n-octylphosphine 63995-75-5,
Sodium triphenylphosphinomono-m-sulfonate 226420-48-0,
(3-Sodiosulfinatophenyl)diphenylphosphine 250788-83-1,
(5-Sodiocarboxy-2-furyl)diphenylphosphine
RL: **CAT (Catalyst use)**; RCT (Reactant); RACT (Reactant or
reagent); USES (Uses)
(**hydrocyanation catalyst** ligand; process for manufacture
of nitriles by **hydrocyanation** of unsatd. compds. with HCN in
ionic liquid solvents)
- IT 1295-35-8, Di(1,5-cyclooctadiene)nickel 7440-02-0, Nickel, uses
7440-05-3, Palladium, uses 7440-06-4, Platinum, uses
RL: **CAT (Catalyst use)**; USES (Uses)
(**hydrocyanation catalyst**; process for manufacture of
nitriles by **hydrocyanation** of unsatd. compds. with HCN in
ionic liquid solvents)
- IT 4553-62-2P, 2-Methylglutaronitrile 17611-82-4P, 2-Ethylsuccinonitrile
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)
(**hydrocyanation** coproduct; process for manufacture of nitriles by
hydrocyanation of unsatd. compds. with HCN in ionic liquid
solvents)
- IT 111-69-3P, Adiponitrile
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP
(Preparation)
(**hydrocyanation** product; process for manufacture of nitriles by
hydrocyanation of unsatd. compds. with HCN in ionic liquid
solvents)
- IT 106-99-0, 1,3-Butadiene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrocyanation substrate**; process for manufacture of
nitriles by **hydrocyanation** of unsatd. compds. with HCN in
ionic liquid solvents)
- IT 75-86-5, Acetone cyanohydrin
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogen cyanide source; process for manufacture of nitriles by

hydrocyanation of unsatd. compds. with HCN in ionic liquid solvents)

- IT 105-60-2P, ϵ -Caprolactam, preparation 124-09-4P, Hexamethylenediamine, preparation
RL: PNU (Preparation, unclassified); PREP (Preparation) (intermediates for; process for manufacture of nitriles by hydrocyanation of unsatd. compds. with HCN in ionic liquid solvents)
- IT 14265-44-2, Phosphate, uses 14797-55-8, Nitrate ion, uses 14874-70-5, Tetrafluoroborate 14996-02-2, Hydrogen sulfate, uses 15529-74-5, Trichlorostannate(1-) 16919-18-9, Hexafluorophosphate 17111-95-4 20461-54-5, Iodide, uses 21340-02-3, Tetrafluoroaluminate 23603-98-7, Trichlorozincate(1-) 24959-67-9, Bromide, uses 98837-98-0, Bis(trifluoromethylsulfuryl)imide
RL: NUU (Other use, unclassified); USES (Uses) (ionic solvent anion; process for manufacture of nitriles by hydrocyanation of unsatd. compds. with HCN in ionic liquid solvents)
- IT 45470-32-4, 1,3-Dimethylimidazolium 65086-10-4, 1,2,3-Trimethylimidazolium 80432-08-2, 1-Butyl-3-methylimidazolium 108203-89-0, 1-Butyl-2,3-dimethylimidazolium
RL: NUU (Other use, unclassified); USES (Uses) (ionic solvent cation; process for manufacture of nitriles by hydrocyanation of unsatd. compds. with HCN in ionic liquid solvents)
- IT 21324-39-0, Sodium hexafluorophosphate 79917-90-1, 1-Butyl-3-methylimidazolium chloride 90076-65-6, Lithium bis(trifluoromethylsulfonyl)amide 98892-75-2, 1-Butyl-2,3-dimethylimidazolium chloride
RL: RCT (Reactant); RACT (Reactant or reagent) (ionic solvent precursor; process for manufacture of nitriles by hydrocyanation of unsatd. compds. with HCN in ionic liquid solvents)
- IT 174899-83-3P, 1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide 227617-70-1P, 1-Butyl-2,3-dimethylimidazolium hexafluorophosphate 350493-08-2P, 1-Butyl-2,3-dimethylimidazolium bis(trifluoromethylsulfonyl)amide
RL: IMF (Industrial manufacture); NUU (Other use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses) (ionic solvent; process for manufacture of nitriles by hydrocyanation of unsatd. compds. with HCN in ionic liquid solvents)
- IT 960-71-4, Triphenylborane 1078-58-6, Diphenylzinc 7646-79-9, Cobalt dichloride, uses 7646-85-7, Zinc chloride, uses 54010-75-2, Zinc triflate 128008-30-0, Indium triflate
RL: CAT (Catalyst use); USES (Uses) (isomerization cocatalyst; process for manufacture of nitriles by hydrocyanation of unsatd. compds. with HCN in ionic liquid solvents)
- IT 592-51-8P, 4-Pentenitrile 4635-87-4P, 3-Pentenitrile
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (isomerization product and hydrocyanation substrate ; process for manufacture of nitriles by hydrocyanation of unsatd. compds. with HCN in ionic liquid solvents)
- IT 16529-56-9, 2-Methyl-3-butenitrile
RL: RCT (Reactant); RACT (Reactant or reagent) (isomerization substrate; process for manufacture of nitriles by hydrocyanation of unsatd. compds. with HCN in ionic liquid solvents)

IT 60-29-7, Diethyl ether, uses 108-20-3, Diisopropyl ether 108-88-3, Toluene, uses 110-54-3, Hexane, uses 111-65-9, Octane, uses 142-82-5, Heptane, uses 598-53-8, Methyl isopropyl ether
RL: NUU (Other use, unclassified); USES (Uses)
(nonpolar cosolvent; process for manufacture of nitriles by **hydrocyanation** of unsatd. compds. with HCN in ionic liquid solvents)

IT 74-90-8, Hydrogen cyanide, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(process for manufacture of nitriles by **hydrocyanation** of unsatd. compds. with HCN in ionic liquid solvents)

IT 13284-42-9P, 2-Pentenitrile
RL: BYP (Byproduct); RCT (Reactant); PREP (Preparation); **RACT (Reactant or reagent)**
(byproduct; process for manufacture of nitriles by **hydrocyanation** of unsatd. compds. with HCN in ionic liquid solvents)

RN 13284-42-9 HCAPLUS
CN 2-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Et-CH=CH-CN

IT 592-51-8P, 4-Pentenitrile 4635-87-4P, 3-Pentenitrile
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(isomerization product and **hydrocyanation substrate** ; process for manufacture of nitriles by **hydrocyanation** of unsatd. compds. with HCN in ionic liquid solvents)

RN 592-51-8 HCAPLUS
CN 4-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

H₂C=CH-CH₂-CH₂-CN

RN 4635-87-4 HCAPLUS
CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Me-CH=CH-CH₂-CN

IT 16529-56-9, 2-Methyl-3-butenitrile
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(isomerization **substrate**; process for manufacture of nitriles by **hydrocyanation** of unsatd. compds. with HCN in ionic liquid solvents)

RN 16529-56-9 HCAPLUS
CN 3-Butenenitrile, 2-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

CN
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Me-CH-CH=CH₂

IT 74-90-8, Hydrogen cyanide, reactions
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(process for manufacture of nitriles by **hydrocyanation** of unsatd.

comps. with HCN in ionic liquid solvents)
RN 74-90-8 HCAPLUS
CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)

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RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L68 ANSWER 6 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2003:93132 HCAPLUS

DN 138:137726

TI Isomerization and **hydrocyanation** of monoolefinic C5-mononitriles
in the presence of Ni(0)-phosphite/phosphonite **catalysts**

IN Bartsch, Michael; Baumann, Robert; Kunsmann-Keitel, Dagmar Pascale;
Haderlein, Gerd; Jungkamp, Tim; Altmayer, Marco; Siegel, Wolfgang

PA BASF AG, Germany

SO Ger. Offen., 18 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	DE 10136488	A1	20030206	DE 2001-10136488	20010727
	TW 570839	B	20040111	TW 2002-91115419	20020711
	CA 2454912	AA	20030213	CA 2002-2454912	20020716
	WO 2003011457	A1	20030213	WO 2002-EP7888	20020716
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	EP 1414567	A1	20040506	EP 2002-791454	20020716
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
	BR 2002011455	A	20040817	BR 2002-11455	20020716
	CN 1535179	A	20041006	CN 2002-814769	20020716
	JP 2004535929	T2	20041202	JP 2003-516681	20020716
	US 2004176622	A1	20040909	US 2004-484169	20040120
PRAI	DE 2001-10136488	A	20010727		
	WO 2002-EP7888	W	20020716		

OS MARPAT 138:137726

AB Monoolefinic C5-mononitriles, e.g., 2-methyl-3-butenenitrile (readily available from **hydrocyanation** of 1,3-butadiene), was isomerized into a mixture of linear mononitrile, e.g., 3-pentenitrile (main) with improved selectivity in the presence of Ni(0) complexes with chelating bisphosphite or bisphosphonite ligands. The pentenenitrile isomers can be further **hydrocyanated** with HCN to the corresponding dinitriles, e.g., adiponitrile, with the same **catalysts** and ZnCl₂

promoter.

IC ICM B01J031-22
ICS B01J031-24; C07C253-10; C07B043-08

CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 67

ST monoolefinic nitrile isomerization **hydrocyanation** dinitrile
manuf; nickel phosphite **catalyst** nitrile isomerization
hydrocyanation; phosphonite nickel **catalyst** nitrile
isomerization **hydrocyanation**

IT **Hydrocyanation catalysts**
Isomerization **catalysts**
(**catalysts** for isomerization and **hydrocyanation** of
nitriles)

IT **Hydrocyanation**
Isomerization
(production of dinitrile monomers from olefinic mononitriles by
catalytic isomerization and hydrocycnation)

IT Nitriles, preparation
RL: IMF (Industrial manufacture); PREP (Preparation)
(production of dinitrile monomers from olefinic mononitriles by
catalytic isomerization and hydrocycnation)

IT 1295-35-8, Bis(1,5-cyclooctadienyl)nickel
RL: CAT (**Catalyst use**); USES (Uses)
(**catalyst** precursor; **catalysts** for isomerization
and **hydrocyanation** of nitriles)

IT 7646-85-7, Zinc chloride, uses
RL: CAT (**Catalyst use**); USES (Uses)
(**catalyst promoter**; **catalysts** for
isomerization and **hydrocyanation** of nitriles)

IT 620-38-2D, Tris(m-Tolyl)phosphite, complex with nickel 620-42-8D,
p-Tolylphosphite, complex with nickel 7440-02-0D, Nickel, complexes with
phosphite ligands 179259-60-0D, complex with nickel 220472-84-4D,
complex with nickel 494227-34-8D, complex with nickel
RL: CAT (**Catalyst use**); USES (Uses)
(**catalysts** for isomerization and **hydrocyanation** of
nitriles)

IT 111-69-3P, Adipodinitrile 16529-66-1P, trans-3-Pentenitrile
16545-78-1P, cis-3-Pentenitrile 20068-02-4P, cis-2-Methyl-2-
butenenitrile 25899-50-7P, cis-2-Pentenitrile 26294-98-4P,
trans-2-Pentenitrile 28906-50-5P, Methylglutaronitrile 30574-97-1P,
trans-2-Methyl-2-butenitrile
RL: IMF (Industrial manufacture); PREP (Preparation)
(production of dinitrile monomers from olefinic mononitriles by
catalytic isomerization and hydrocycnation)

IT 4635-87-4P, 3-Pentenitrile
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation);
RACT (Reactant or reagent)
(production of dinitrile monomers from olefinic mononitriles by
catalytic isomerization and hydrocycnation)

IT 74-90-8, Hydrocyanic acid, reactions 106-99-0, 1,3-Butadiene,
reactions 16529-56-9, 2-Methyl-3-butenitrile
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(production of dinitrile monomers from olefinic mononitriles by
catalytic isomerization and hydrocycnation)

IT 4635-87-4P, 3-Pentenitrile
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation);
RACT (Reactant or reagent)
(production of dinitrile monomers from olefinic mononitriles by
catalytic isomerization and hydrocycnation)

RN 4635-87-4 HCAPLUS

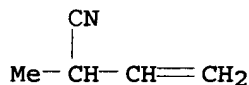
CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 74-90-8, Hydrocyanic acid, reactions 16529-56-9,
2-Methyl-3-butenitrile
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(production of dinitrile monomers from olefinic mononitriles by
catalytic isomerization and hydrocyanation)
RN 74-90-8 HCAPLUS
CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)



RN 16529-56-9 HCAPLUS
CN 3-Butenenitrile, 2-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L68 ANSWER 7 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:142589 HCAPLUS
DN 136:184268
TI Synthesis of dinitrile monomers from olefinic mononitriles by
catalytic isomerization and **hydrocyanation**
IN Bartsch, Michael; Kunsmann-Keitel, Dagmar Pascale; Baumann, Robert;
Haderlein, Gerd; Siegel, Wolfgang
PA Basf Aktiengesellschaft, Germany
SO PCT Int. Appl., 24 pp.
CODEN: PIXXD2
DT Patent
LA German
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002013964	A2	20020221	WO 2001-EP8522	20010724
	WO 2002013964	A3	20020718		
	W:				
	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				
	CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,				
	GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,				
	LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT,				
	RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US,				
	UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,				
	DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,				
	BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
	DE 10038037	A1	20020418	DE 2000-10038037	20000802
	AU 2001082012	A5	20020225	AU 2001-82012	20010724
PRAI	DE 2000-10038037	A	20000802		
	WO 2001-EP8522	W	20010724		

- OS MARPAT 136:184268
- AB Branched monoolefinic C5-mononitriles, e.g. 2-methyl-3-butenenitrile (readily available from **hydrocyanation** of 1,3-butadiene), was isomerized into a mixture of linear mononitriles, e.g. 3-pentenitrile (main), in the presence of an 1,2-benzo-linked bisphosphite-Ni(0) **catalyst**. The pentenenitrile isomers can be further **hydrocyanated** with HCN to the corresponding dinitriles, e.g. adiponitrile, with the same **catalysts** and ZnCl₂ **promoter** in an anti-Markovnikov addition fashion.
- IC ICM B01J031-18
ICS C07F015-04; C07F009-48; C07F009-145; C07F009-46; C07F009-6574; C07C253-10
- CC 35-2 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 67
- ST monoolefinic nitrile isomerization **hydrocyanation** dinitrile manuf; phosphite nickel **catalysts** nitrile isomerization **hydrocyanation**
- IT **Hydrocyanation**
Hydrocyanation catalysts
Isomerization
Isomerization **catalysts**
(production of dinitrile monomers from olefinic mononitriles by **catalytic** isomerization and **hydrocyanation**)
- IT Nitriles, preparation
RL: IMF (Industrial manufacture); PREP (Preparation)
(production of dinitrile monomers from olefinic mononitriles by **catalytic** isomerization and **hydrocyanation**)
- IT 1295-35-8, Bis(1,5-cyclooctadienyl)nickel
RL: CAT (Catalyst use); USES (Uses)
(**catalyst** precursor; **catalysts** for isomerization and **hydrocyanation** of nitriles)
- IT 7646-85-7, Zinc dichloride, uses
RL: CAT (Catalyst use); USES (Uses)
(**catalyst promoter**; **catalysts** for isomerization and **hydrocyanation** of nitriles)
- IT 7440-02-0D, Nickel, complexes with phosphite ligands 399573-32-1D, complex with Ni 399573-34-3D, complex with Ni 399573-36-5D, complex with Ni 399573-38-7D, complex with Ni 399573-40-1D, complex with Ni 399573-42-3D, complex with Ni
RL: CAT (Catalyst use); USES (Uses)
(**catalysts** for isomerization and **hydrocyanation** of nitriles)
- IT 74-90-8, Hydrocyanic acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrocyanation**; production of dinitrile monomers from olefinic mononitriles by **catalytic** isomerization and **hydrocyanation**)
- IT 111-69-3P, Adiponitrile 592-51-8P, 4-Pentenitrile 4403-61-6P, 2-Methyl-2-butenenitrile 28906-50-5P, Methylglutaronitrile
RL: IMF (Industrial manufacture); PREP (Preparation)
(production of dinitrile monomers from olefinic mononitriles by **catalytic** isomerization and **hydrocyanation**)
- IT 16529-66-1P, trans-3-Pentenitrile
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)
(production of dinitrile monomers from olefinic mononitriles by **catalytic** isomerization and **hydrocyanation**)
- IT 16529-56-9, 2-Methyl-3-butenenitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(production of dinitrile monomers from olefinic mononitriles by

catalytic isomerization and hydrocyanation)
 IT 74-90-8, Hydrocyanic acid, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrocyanation; production of dinitrile monomers from olefinic mononitriles by **catalytic isomerization and hydrocyanation**)
 RN 74-90-8 HCAPLUS
 CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)

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IT 592-51-8P, 4-Pentenitrile
 RL: IMF (Industrial manufacture); PREP (Preparation)
 (production of dinitrile monomers from olefinic mononitriles by **catalytic isomerization and hydrocyanation**)
 RN 592-51-8 HCAPLUS
 CN 4-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

$$\text{H}_2\text{C}=\text{CH}-\text{CH}_2-\text{CH}_2-\text{CN}$$

IT 16529-56-9, 2-Methyl-3-butenitrile
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (production of dinitrile monomers from olefinic mononitriles by **catalytic isomerization and hydrocyanation**)
 RN 16529-56-9 HCAPLUS
 CN 3-Butenenitrile, 2-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

CN
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 Me-CH-CH=CH₂

L68 ANSWER 8 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2000:238077 HCAPLUS
 DN 132:280878
 TI Insoluble **promoters** for nickel-catalyzed **hydrocyanation** of monoolefins
 IN Clarkson, Lucy Mary; Herron, Norman; Kalb, William C.; McKinney, Ronald James; Moran, Edward Francis, Jr.
 PA E. I. Du Pont de Nemours & Co., USA
 SO U.S., 10 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 6048996	A	20000411	US 1999-383898	19990826
	TW 528743	B	20030421	TW 2000-89112277	20000622
	CA 2381057	AA	20010301	CA 2000-2381057	20000718
	WO 2001014321	A1	20010301	WO 2000-US19385	20000718

W: BR, CA, CN, ID, JP, KR, MX, SG

RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE

BR 2000013810	A	20020423	BR 2000-13810	20000718
EP 1212293	A1	20020612	EP 2000-950380	20000718
EP 1212293	B1	20050223		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
IE, FI, CY

JP 2003507451	T2	20030225	JP 2001-518411	20000718
PRAI US 1999-383898	A	19990826		
WO 2000-US19385	W	20000718		

AB An improved process for converting an acyclic monoolefin to its corresponding terminal organonitrile by reacting the monoolefin with hydrogen cyanide in the presence of zero-valent nickel, a phosphite ligand, and an insol. Lewis acid **promoter** is disclosed.

IC ICM C07C253-10

INCL 558338000

CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)

Section cross-reference(s): 67

ST olefin **hydrocyanation nickel catalyst**; nitrile manuf
nickel catalyst; insol **promoter nickel**
hydrocyanation catalyst

IT Polyoxyalkylenes, uses

RL: **CAT (Catalyst use)**; USES (Uses)
(fluorine- and sulfo-containing, ionomers; insol. **promoters** for
nickel-catalyzed hydrocyanation of monoolefins)

IT Polyoxyalkylenes, uses

RL: **CAT (Catalyst use)**; USES (Uses)
(fluorine-containing, sulfo-containing, ionomers; insol. **promoters**
for **nickel-catalyzed hydrocyanation** of monoolefins)

IT **Hydrocyanation catalysts**

(insol. **promoters** for **nickel-catalyzed**
hydrocyanation of monoolefins)

IT Aluminosilicates, uses

Oxides (inorganic), uses

Zeolites (synthetic), uses

RL: **CAT (Catalyst use)**; USES (Uses)
(insol. **promoters** for **nickel-catalyzed**
hydrocyanation of monoolefins)

IT Nitriles, preparation

RL: IMF (Industrial manufacture); PREP (Preparation)
(insol. **promoters** for **nickel-catalyzed**
hydrocyanation of monoolefins)

IT Alkenes, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
(insol. **promoters** for **nickel-catalyzed**
hydrocyanation of monoolefins)

IT Clays, uses

RL: **CAT (Catalyst use)**; USES (Uses)
(montmorillonitic; insol. **promoters** for **nickel-**
catalyzed hydrocyanation of monoolefins)

IT Fluoropolymers, uses

Fluoropolymers, uses

RL: **CAT (Catalyst use)**; USES (Uses)
(polyoxyalkylene-, sulfo-containing, ionomers; insol. **promoters**
for **nickel-catalyzed hydrocyanation** of monoolefins)

IT Ionomers

RL: **CAT (Catalyst use)**; USES (Uses)
(polyoxyalkylenes, fluorine- and sulfo-containing; insol. **promoters**
for **nickel-catalyzed hydrocyanation** of monoolefins)

IT Lewis acids

- RL: CAT (Catalyst use); USES (Uses)
(promoter; insol. promoters for nickel-catalyzed hydrocyanation of monoolefins)
- IT Rare earth metals, uses
Transition metals, uses
RL: CAT (Catalyst use); USES (Uses)
(reaction products with polystyrene; insol. promoters for nickel-catalyzed hydrocyanation of monoolefins)
- IT Clays, uses
RL: CAT (Catalyst use); USES (Uses)
(silicoaluminate; insol. promoters for nickel-catalyzed hydrocyanation of monoolefins)
- IT 1295-35-8 1309-37-1, Iron oxide (Fe₂O₃), uses 1312-81-8, Lanthanum oxide 1314-13-2, Zinc oxide (ZnO), uses 1314-23-4, Zirconium oxide (ZrO₂), uses 1318-93-0, Montmorillonite, uses 7429-90-5D, Aluminum, reaction products with polystyrene, uses 7429-91-6D, Dysprosium, reaction products with perfluorosulfonic acid resin, uses 7439-89-6D, Iron, reaction products with perfluorosulfonic acid resin, uses 7439-91-0D, Lanthanum, reaction products with perfluorosulfonic acid resin, uses 7439-94-3D, Lutetium, reaction products with perfluorosulfonic acid resin, uses 7439-96-5D, Manganese, reaction products with perfluorosulfonic acid resin, uses 7440-00-8D, Neodymium, reaction products with perfluorosulfonic acid resin, uses 7440-02-0D, Nickel, zerovalent compds., uses 7440-10-0D, Praseodymium, reaction products with perfluorosulfonic acid resin, uses 7440-15-5D, Rhenium, reaction products with polystyrene, uses 7440-19-9D, Samarium, reaction products with perfluorosulfonic acid resin, uses 7440-25-7D, Tantalum, reaction products with polystyrene, uses 7440-27-9D, Terbium, reaction products with perfluorosulfonic acid resin, uses 7440-30-4D, Thulium, reaction products with perfluorosulfonic acid resin, uses 7440-31-5D, Tin, reaction products with polystyrene, uses 7440-33-7D, Tungsten, reaction products with polystyrene, uses 7440-42-8D, Boron, reaction products with polystyrene, uses 7440-43-9D, Cadmium, reaction products with polystyrene, uses 7440-45-1D, Cerium, reaction products with perfluorosulfonic acid resin, uses 7440-48-4D, Cobalt, reaction products with perfluorosulfonic acid resin, uses 7440-52-0D, Erbium, reaction products with perfluorosulfonic acid resin, uses 7440-53-1D, Europium, reaction products with perfluorosulfonic acid resin, uses 7440-54-2D, Gadolinium, reaction products with perfluorosulfonic acid resin, uses 7440-55-3D, Gallium, reaction products with polystyrene, uses 7440-56-4D, Germanium, reaction products with polystyrene, uses 7440-58-6D, Hafnium, reaction products with polystyrene, uses 7440-60-0D, Holmium, reaction products with perfluorosulfonic acid resin, uses 7440-64-4D, Ytterbium, reaction products with perfluorosulfonic acid resin, uses 7440-66-6D, Zinc, reaction products with perfluorosulfonic acid resin, uses 7440-66-6D, Zinc, reaction products with polystyrene, uses 7440-74-6D, Indium, reaction products with polystyrene, uses 7782-91-4, Molybdic acid 7783-49-5D, Zinc fluoride (ZnF₂), reaction products with perfluorosulfonic acid resin 7783-70-2D, Antimony pentafluoride, reaction products with perfluorosulfonic acid resin 7784-18-1D, Aluminum fluoride (AlF₃), reaction products with perfluorosulfonic acid resin 9003-53-6D, Polystyrene, metal cation-containing 11105-11-6, Tungstic acid 11115-92-7, Iron hydroxide oxide 13463-67-7, Titanium dioxide, uses 14940-41-1 35884-66-3 37349-30-7, Niobic acid
RL: CAT (Catalyst use); USES (Uses)
(insol. promoters for nickel-catalyzed hydrocyanation of monoolefins)
- IT 111-69-3P, Adiponitrile 17611-82-4P, Ethylsuccinonitrile 28906-50-5P, Methylglutaronitrile

RL: IMF (Industrial manufacture); PREP (Preparation)
(insol. promoters for nickel-catalyzed
hydrocyanation of monoolefins)
IT 74-90-8, Hydrogen cyanide, reactions 592-51-8,
4-Pentenitrile 4635-87-4, 3-Pentenitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(insol. promoters for nickel-catalyzed
hydrocyanation of monoolefins)
IT 1344-28-1, γ -Alumina, uses
RL: CAT (Catalyst use); USES (Uses)
(γ -, acidic; insol. promoters for nickel-
catalyzed hydrocyanation of monoolefins)
IT 74-90-8, Hydrogen cyanide, reactions 592-51-8,
4-Pentenitrile 4635-87-4, 3-Pentenitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(insol. promoters for nickel-catalyzed
hydrocyanation of monoolefins)
RN 74-90-8 HCAPLUS
CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)

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RN 592-51-8 HCAPLUS
CN 4-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 4635-87-4 HCAPLUS
CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L68 ANSWER 9 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:788781 HCAPLUS

DN 130:26464

TI Process for the hydrocyanation of olefins using bidentate
phosphite ligands and zero-valent nickel catalyst systems which
enable facile nitrile product and catalyst separation

IN Bunel, Emilio Enrique; McNulty, Kenneth C.

PA E. I. Du Pont de Nemours & Co., USA

SO U.S., 10 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

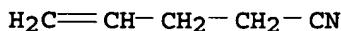
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5847191	A	19981208	US 1997-902438	19970729
	TW 580490	B	20040321	TW 1998-87111507	19980715

WO 9906359 A1 19990211 WO 1998-US15621 19980728
W: CA, CN, ID, JP, KR, SG
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE
EP 1001928 A1 20000524 EP 1998-936024 19980728
EP 1001928 B1 20050406
R: BE, DE, ES, FR, GB, IT, NL
JP 2001512097 T2 20010821 JP 2000-505121 19980728
JP 3380543 B2 20030224
CA 2291640 C 20040921 CA 1998-2291640 19980728
CA 2291640 AA 19990211
PRAI US 1997-902438 A 19970729
WO 1998-US15621 W 19980728
OS MARPAT 130:26464
AB Nitriles (e.g., adiponitrile) are prepared in high yield and selectivity by the **hydrocyanation** of an alkene (e.g., 3-pentenitrile) in a two-phase process solvent (e.g., liquid HCN extracted with pentane) with HCN in the presence of a Lewis acid **promoter** (e.g., ZnCl₂) and a **catalyst** system comprising zero-valent nickel [e.g., Nickel bis(cyclooctadiene)] and an aromatic-substituted bidentate phosphite ligand (PR₂)NR₁ [R, R₁ = organic residues which may be the same or different and where the R or R' contain at ≥1 C₉₋₄₀ aliphatic group positioned as a tail extending away from the primary ligand structure rendering the ligand lipophilic; n = 1, 2].
IC ICM C07C253-00
INCL 558338000
CC 45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes)
Section cross-reference(s): 23, 29, 35, 48, 67
ST **hydrocyanation catalyst** adiponitrile manuf; nickel bidentate phosphite **hydrocyanation catalyst** alkene conversion nitrile; pentenenitrile **hydrocyanation** adiponitrile manuf; Lewis acid **catalyst promoter** manuf adiponitrile
IT **Hydrocyanation catalysts**
(bidentate phosphite ligands and zero-valent nickel compds. with Lewis acid **promoters** for the conversion of alkenes into nitriles)
IT Ligands
RL: CAT (Catalyst use); USES (Uses)
(bidentate, phosphites; bidentate phosphite ligands and zero-valent nickel **catalyst** systems for the **hydrocyanation** of olefins into nitriles)
IT Lewis acids
RL: CAT (Catalyst use); USES (Uses)
(**catalyst promoters** for the **hydrocyanation** of olefins using bidentate phosphite ligands and zero-valent nickel **catalyst** systems which enable facile product and **catalyst** separation)
IT Nitriles, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(dinitriles; process for the **hydrocyanation** of olefins using bidentate phosphite ligands and zero-valent nickel **catalyst** systems which enable facile product and **catalyst** separation)
IT **Hydrocyanation**
(of alkenes in the manuf of nitriles)
IT Nitriles, preparation
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for the **hydrocyanation** of olefins using bidentate phosphite ligands and zero-valent nickel **catalyst** systems which enable facile product and **catalyst** separation)

- IT Alkadienes
Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for the **hydrocyanation** of olefins using bidentate phosphite ligands and zero-valent nickel **catalyst** systems which enable facile product and **catalyst** separation)
- IT 7440-02-0D, Nickel, derivs. or complexes, uses 216220-59-6 216220-64-3 216220-69-8
RL: CAT (Catalyst use); USES (Uses)
(process for the **hydrocyanation** of olefins using bidentate phosphite ligands and zero-valent nickel **catalyst** systems which enable facile nitrile product and **catalyst** separation)
- IT 111-69-3P, Adiponitrile
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(process for the **hydrocyanation** of olefins using bidentate phosphite ligands and zero-valent nickel **catalyst** systems which enable facile nitrile product and **catalyst** separation)
- IT 74-90-8, Hydrogen cyanide, reactions 88-69-7, 2-Isopropylphenol 90-05-1, Guaiacol 95-48-7, reactions 112-13-0, Decanoyl chloride 592-51-8, 4-Pentenitrile 1069-08-5, Dichloro(diethylamino)phosphine 4635-87-4, 3-Pentenitrile 4635-87-4D, 3-Pentenitrile, alkyl derivs.
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for the **hydrocyanation** of olefins using bidentate phosphite ligands and zero-valent nickel **catalyst** systems which enable facile nitrile product and **catalyst** separation)
- IT 602-09-5P, [1,1'-Binaphthalene]-2,2'-diol 13990-86-8P 22277-50-5P 59832-97-2P 66475-96-5P 66476-01-5P 109250-83-1P 109250-85-3P 110025-88-2P 216220-58-5P 216220-62-1P 216220-65-4P 216220-66-5P 216220-67-6P 216220-68-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for the **hydrocyanation** of olefins using bidentate phosphite ligands and zero-valent nickel **catalyst** systems which enable facile nitrile product and **catalyst** separation)
- IT 74-90-8, Hydrogen cyanide, reactions 592-51-8, 4-Pentenitrile 4635-87-4, 3-Pentenitrile 4635-87-4D, 3-Pentenitrile, alkyl derivs.
RL: RCT (Reactant); RACT (Reactant or reagent)
(process for the **hydrocyanation** of olefins using bidentate phosphite ligands and zero-valent nickel **catalyst** systems which enable facile nitrile product and **catalyst** separation)
- RN 74-90-8 HCAPLUS
CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)

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RN 592-51-8 HCAPLUS
CN 4-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 4635-87-4 HCAPLUS

CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Me-CH=CH-CH₂-CN

RN 4635-87-4 HCAPLUS

CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Me-CH=CH-CH₂-CN

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L68 ANSWER 10 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:430104 HCAPLUS

DN 129:89455

TI Perfluoroalkanesulfonates, their preparation and use as **catalysts**
for increasing fluorine content of halogenated hydrocarbons and as
promoter for **hydrocyanation** of olefins

IN Cicha, Walter Vladimir; Kornath, Andreas Josef; McKinney, Ronald James;
Rao, V. N. Mallikarjuna; Thrasher, Joseph Stuart; Waterfeld, Alfred

PA E. I. Du Pont de Nemours & Co., USA

SO U.S., 6 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5773637	A	19980630	US 1996-708997	19960906
PRAI	US 1996-708997		19960906		

OS MARPAT 129:89455

AB A process is disclosed for preparing a perfluoroalkanesulfonate compound $\text{RaMXb-cOg}[(\text{SO}_3)\text{d}(\text{Rf})\text{e}]_c$. This process involves reacting a reagent of the formula RaMXbOg and a second reagent $\text{R}'\text{xE}[(\text{SO}_3)\text{d}(\text{Rf})\text{e}]_y$, where R is selected from C1-C6 alkyl, C1-C6 perfluoroalkyl, cyclopentadienyl, Ph and C6F5; M is selected from transition metals of Groups 3-12, Main group elements of Group 13-16 and lanthanide metals; X is selected from F, Cl and Br; Rf is selected from ChF_{2h+1} , ChF_{2h} , wherein $h = 1-10$, C6F5, C6F4(CF2)_{2i} wherein $i = 0-6$, provided that when E is B, Rf is selected from $\text{ChF}_{2h'+1}$, wherein $h' = 1-10$, C6F5; R' is selected from CjH_{2j+1} , wherein $j = 1-4$, and Ph; E = B or Si; a = 0-3; b = 2-6; c = 1-6; d = 1 to 3; e = 1-4; g = 0-1; x = 0-3; and y = 1-3. Novel perfluoroalkanesulfonates provided include $\text{TaCl}_4(\text{SO}_3\text{CF}_3)$, $\text{Ta}_2\text{F}_5(\text{SO}_3\text{CF}_3)_5$, $\text{TaF}_2(\text{SO}_3\text{CF}_3)_3$, $\text{NbCl}_4(\text{SO}_3\text{CF}_3)$, $\text{NbF}_3(\text{SO}_3\text{CF}_3)_2$, $\text{NbF}_2(\text{SO}_3\text{CF}_3)_3$, $\text{TiF}_2(\text{SO}_3\text{CF}_3)_2$, $\text{TiF}_3(\text{SO}_3\text{CF}_3)$, $\text{Ti}_5\text{Cl}_{17}(\text{SO}_3\text{CF}_3)_3$, $\text{Ti}_5\text{Cl}_{12}(\text{SO}_3\text{CF}_3)_3$, $\text{BiF}_4(\text{SO}_3\text{CF}_3)$, $\text{BiF}_2(\text{SO}_3\text{CF}_3)_3$, $\text{Bi}(\text{SO}_3\text{CF}_3)_3$, $\text{Pb}_4\text{F}_5(\text{SO}_3\text{CF}_3)_3$, $\text{Pb}_5\text{F}_{17}(\text{SO}_3\text{CF}_3)_3$, $\text{Sn}_2\text{F}_7(\text{SO}_3\text{CF}_3)$, $\text{TeF}_2(\text{SO}_3\text{CF}_3)_2$, $\text{ZrCl}(\text{SO}_3\text{CF}_3)_3$, $\text{CrF}_2(\text{SO}_3\text{CF}_3)$, $\text{AsF}(\text{SO}_3\text{CF}_3)_2$, $\text{AsF}_2(\text{SO}_3\text{CF}_3)_2$, $\text{As}(\text{SO}_3\text{CF}_3)_3$, $\text{BiF}_2(\text{SO}_3\text{CF}_3)$, $\text{SbF}_2(\text{SO}_3\text{CF}_3)$, $\text{SbF}_3(\text{SO}_3\text{CF}_3)_2$, $\text{Sb}_2\text{F}(\text{SO}_3\text{CF}_3)_5$, $\text{Ge}_5\text{F}_{13}(\text{SO}_3\text{CF}_3)_7$, $\text{MoCl}_2(\text{SO}_3\text{CF}_3)_2$, $\text{AsF}_4(\text{SO}_3\text{CF}_3)$, $\text{HfCl}(\text{SO}_3\text{CF}_3)_3$, $\text{V}_2\text{F}_7(\text{SO}_3\text{CF}_3)$, $\text{VO}(\text{SO}_3\text{CF}_3)_3$, $\text{VOF}(\text{SO}_3\text{CF}_3)_2$, and $\text{In}_2\text{Cl}_3(\text{SO}_3\text{CF}_3)_3$. The perfluoroalkanesulfonates are useful as **catalysts** for increasing the F content of halogenated hydrocarbons and as **promoters** for **hydrocyanation** of olefins. Thus, reaction of TiF_4 with Me_3SiOTf for 18 h at 25° afforded $\text{TiF}_2(\text{OTf})_2$. Reaction of $\text{CCl}_3\text{CH}_2\text{CCl}_3$ with HF in an autoclave **catalyzed** by $\text{TiF}_2(\text{OTf})_2$ afforded mostly $\text{CF}_3\text{CH}_2\text{CCl}_2\text{F}$ and lesser amts. of $\text{CF}_3\text{CH}_2\text{CClF}_2$ and

- CF3CH2CCl3. **Hydrocyanation** of MeCH:CHCH2CN with HCN was achieved in the presence of Ni(COD)2 (COD = 1,5-cyclooctadiene) **catalyst**, a diphosphite ligand, and Sn(OTf)4 **promoter** under an inert atmosphere of N2. Products were dinitriles (including methylglutaronitrile and ethylsuccinonitrile) and adiponitrile.
- IC ICM C07F009-00
ICS C07F007-00; C07F009-70; C07F007-22
- INCL 556001000
- CC 78-7 (Inorganic Chemicals and Reactions)
Section cross-reference(s): 45, 67
- ST perfluoroalkanesulfonate prepn **catalyst** fluorination
hydrocyanation; fluorination **catalyst** metal metalloid
perfluoroalkanesulfonate; **hydrocyanation catalyst**
metal metalloid perfluoroalkanesulfonate; olefin **hydrocyanation**
perfluoroalkanesulfonate **promoter**; hydrocarbon halo fluorination
perfluoroalkanesulfonate **catalyst**
- IT Sulfonates
RL: **CAT (Catalyst use)**; SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)
(alkanesulfonates, perfluoroalkanesulfonates; preparation of metal and
metalloid perfluoroalkanesulfonates as fluorination **catalysts**
for halohydrocarbons and as **promoters** for
hydrocyanation of olefins)
- IT Hydrocarbons, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(halo; fluorination of halogenated hydrocarbons **catalyzed** by
perfluoroalkanesulfonates)
- IT Alkenes, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrocyanation** of olefins **promoted** by
perfluoroalkanesulfonates)
- IT Fluorination **catalysts**
(metal and metalloid perfluoroalkanesulfonates as **catalysts**
for increasing F content of halogenated hydrocarbons)
- IT **Hydrocyanation catalysts**
(metal and metalloid perfluoroalkanesulfonates as **promoters**
for **hydrocyanation** of olefins)
- IT 1295-35-8, Bis(1,5-cyclooctadiene)nickel
RL: **CAT (Catalyst use)**; USES (Uses)
(cocatalyst with diphosphite ligand, for **hydrocyanation** of
olefin in presence of perfluoroalkanesulfonate **promoter**)
- IT 121627-17-6
RL: **CAT (Catalyst use)**; USES (Uses)
(cocatalyst with nickel complex, for **hydrocyanation** of olefin
in presence of perfluoroalkanesulfonate **promoter**)
- IT 3607-78-1, 1,1,1,3,3,3-Hexachloropropane 7664-39-3, Hydrogen fluoride,
reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorination of halo hydrocarbon with hydrogen fluoride
catalyzed by perfluoroalkanesulfonate)
- IT 460-92-4P 7125-84-0P 64712-27-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(fluorination of halo hydrocarbon with hydrogen fluoride
catalyzed by perfluoroalkanesulfonate)
- IT 7550-45-0, Titanium tetrachloride, reactions 7705-07-9, Titanium
trichloride, reactions 7721-01-9, Tantalum pentachloride 7783-46-2,
Lead difluoride 7783-56-4, Antimony trifluoride 7783-58-6, Germanium
tetrafluoride 7783-59-7, Lead tetrafluoride 7783-62-2, Tin
tetrafluoride 7783-63-3, Titanium tetrafluoride 7783-68-8, Niobium
pentafluoride 7783-71-3, Tantalum pentafluoride 7784-35-2, Arsenic

trifluoride 7784-36-3, Arsenic pentafluoride 7787-61-3, Bismuth
trifluoride 10026-11-6, Zirconium tetrachloride 10026-12-7, Niobium
pentachloride 10049-16-8, Vanadium tetrafluoride 13320-71-3,
Molybdenum tetrachloride 13499-05-3, Hafnium tetrachloride 13709-31-4,
Vanadyl trifluoride 15192-26-4, Tellurium tetrafluoride 22519-64-8,
Indium trichloride tetrahydrate 27607-77-8, Trimethylsilyl triflate
72500-12-0 179179-65-8, Chromium trifluoride tetrahydrate
RL: RCT (Reactant); RACT (Reactant or reagent)
(for preparation of perfluoroalkanesulfonate)

IT 62086-02-6
RL: CAT (Catalyst use); USES (Uses)
(hydrocyanation of olefin in presence of
perfluoroalkanesulfonate promoter)

IT 74-90-8, Hydrogen cyanide, reactions 4635-87-4,
3-Pentenitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrocyanation of olefin in presence of
perfluoroalkanesulfonate promoter)

IT 111-69-3P, Adiponitrile 17611-82-4P, Ethylsuccinonitrile 28906-50-5P,
Methylglutaronitrile
RL: SPN (Synthetic preparation); PREP (Preparation)
(hydrocyanation of olefin in presence of
perfluoroalkanesulfonate promoter)

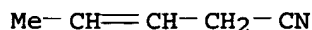
IT 7439-92-1DP, Lead, fluoro triflate cluster complexes, preparation
7439-98-7DP, Molybdenum, chloro triflate pentanuclear cluster, preparation
7440-25-7DP, Tantalum, fluoro triflate binuclear complex, preparation
7440-31-5DP, Tin, fluoro triflate binuclear complex, preparation
7440-32-6DP, Titanium, chloro triflate pentanuclear cluster complexes,
preparation 7440-36-0DP, Antimony, fluoro triflate binuclear complex,
preparation 7440-56-4DP, Germanium, fluoro triflate pentanuclear cluster
complex, preparation 7440-62-2DP, Vanadium, fluoro triflate binuclear
complex, preparation 7440-74-6DP, Indium, chloro triflate binuclear
complex, preparation 81439-30-7P 88189-03-1P, Bismuth triflate
208983-01-1P 208983-02-2P 208983-03-3P 208983-04-4P 208983-05-5P
208983-06-6P 208983-07-7P 208983-08-8P 208983-09-9P 208983-10-2P
208983-11-3P 208983-12-4P 208983-13-5P 208983-14-6P 208983-15-7P
208983-16-8P 208983-17-9P 208983-18-0P 208983-19-1P 208983-20-4P
209159-36-4P 209159-38-6P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)
(preparation of metal and metalloid perfluoroalkanesulfonates as
fluorination catalysts for halohydrocarbons and as
promoters for hydrocyanation of olefins)

IT 74-90-8, Hydrogen cyanide, reactions 4635-87-4,
3-Pentenitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrocyanation of olefin in presence of
perfluoroalkanesulfonate promoter)

RN 74-90-8 HCAPLUS
CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)

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RN 4635-87-4 HCAPLUS
CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L68 ANSWER 11 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:392151 HCAPLUS

DN 125:114201

TI Process for **hydrocyanation** of pentenenitriles, alkylpentenoates, and perfluoroalkylethenes with nickel(0) compounds and bidentate phosphorus ligands as **catalysts** in presence of Lewis acid **promoters**

IN Breikss, Anne I.

PA du Pont de Nemours, E. I., and Co., USA

SO U.S., 12 pp.

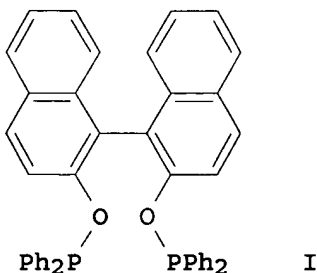
CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5523453	A	19960604	US 1995-408250	<u>19950322</u>
	IN 186815	A	20011117	IN 1996-CA206	19960205
	CA 2214009	AA	19960926	CA 1996-2214009	19960307
	CA 2214009	C	20040224		
	WO 9629303	A1	19960926	WO 1996-US2551	19960307
	W: BR, CA, CN, JP, KR, SG				
	RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
	EP 815073	A1	19980107	EP 1996-908520	19960307
	EP 815073	B1	20010718		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
	CN 1179147	A	19980415	CN 1996-192673	19960307
	CN 1069310	B	20010808		
	JP 10505101	T2	19980519	JP 1996-528423	19960307
	JP 2911608	B2	19990623		
	BR 9607982	A	19980623	BR 1996-7982	19960307
	AT 203233	E	20010815	AT 1996-908520	19960307
PRAI	US 1995-408250	A	19950322		
	WO 1996-US2551	W	19960307		
OS	CASREACT 125:114201; MARPAT 125:114201				
GI					



AB A process for **hydrocyanation** comprises reacting
2-pentenenitrile, 3-pentenenitrile, 4-pentenenitrile, alkyl-3-pentenoate,

alkyl-4-pentenoate, or $CzF2z+1CH:CH2$ ($z = 1-12$) with HCN in the presence of a Lewis acid **promoter** and a **catalyst** comprising a **zero-valent Ni** compound and a bidentate phosphorus ligand, e.g., biaryl diphenylphosphinite ligand I, or an analog. The HCN adds to the double bond primarily in an anti-Markovnikov manner. Thus, **hydrocyanation** of 3-pentenitrile with HCN in the presence of $Ni(COD)_2$ (COD = 1,5-cyclooctadiene), ligand I (preparation given), and $ZnCl_2$ as Lewis acid **promoter** in THF afforded 36.8% adiponitrile, 12.0% methylglutaronitrile, and 1.2% ethylsuccinonitrile as determined by GC anal.

IC ICM C07C253-10

INCL 558338000

CC 23-19 (Aliphatic Compounds)

Section cross-reference(s): 29

ST **hydrocyanation catalyst** nickel bidentate biaryl diphenylphosphinite; phosphinite biaryl bidentate nickel **hydrocyanation catalyst**; phosphorus bidentate ligand nickel **hydrocyanation catalyst**; pentenenitrile **hydrocyanation catalytic**; alkylpentenoate **hydrocyanation catalytic**; pentenoate **hydrocyanation catalytic**; perfluoroalkylethene **hydrocyanation catalytic**; Lewis acid **promoter** nickel **catalyzed hydrocyanation**

IT Perfluorocarbons

RL: RCT (Reactant); RACT (Reactant or reagent)

(C1-12, ethenyl; **hydrocyanation** of pentenenitriles, alkylpentenoates, and perfluoroalkylethenes with nickel(0) compds. and bidentate phosphorus ligands as **catalysts** in presence of Lewis acid **promoters**)

IT **Hydrocyanation catalysts**

(nickel(0) compds. and bidentate phosphorus ligands in presence of Lewis acid **promoters** for pentenenitriles, alkylpentenoates, and perfluoroalkylethenes)

IT **Hydrocyanation**

(of pentenenitriles, alkylpentenoates, and perfluoroalkylethenes with nickel(0) compds. and bidentate phosphorus ligands as **catalysts** in presence of Lewis acid **promoters**)

IT Lewis acids

RL: CAT (Catalyst use); USES (Uses)

(**promoters**, for **hydrocyanation** of pentenenitriles, alkylpentenoates, and perfluoroalkylethenes with nickel(0) compds. and bidentate phosphorus ligands as **catalysts**)

IT Ligands

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(bidentate, phosphorus-containing; **catalysts** with nickel(0) compds. and Lewis acid **promoters** for **hydrocyanation** of pentenenitriles, alkylpentenoates, and perfluoroalkylethenes)

IT 960-71-4, Triphenylboron 1295-35-8, Bis(1,5-cyclooctadiene)nickel 1779-25-5, Chlorodiisobutylaluminum 3238-27-5, Dichloro(octyl)aluminum 6591-30-6, Chlorodiphenylaluminum 7446-70-0, Aluminum trichloride, uses 7447-39-4, Copper dichloride, uses 7550-45-0, Titanium tetrachloride, uses 7646-79-9, Cobalt dichloride, uses 7646-85-7, Zinc dichloride, uses 7699-45-8, Zinc dibromide 7705-07-9, Titanium trichloride, uses 7705-08-0, Iron trichloride, uses 7718-98-1, Vanadium trichloride 7721-01-9, Tantalum pentachloride 7733-02-0, Zinc sulfate 7758-89-6, Cuprous chloride 7773-01-5, Manganese dichloride 7783-86-0, Iron diiodide 10026-11-6, Zirconium tetrachloride 10026-12-7, Niobium pentachloride 10049-05-5, Chromium dichloride 10099-58-8, Lanthanum trichloride 10108-64-2, Cadmium dichloride 10139-47-6, Zinc diiodide 10241-05-1, Molybdenum pentachloride 10361-82-7, Samarium trichloride

10361-84-9, Scandium trichloride 10361-92-9, Yttrium trichloride
13596-35-5, Rhenium pentachloride 15238-00-3, Cobalt diiodide
20717-86-6, Chlorotriisopropoxytitanium 27607-85-8, Triphenyltin
triflate 29537-91-5, Triphenyltin tosylate 31011-57-1,
Tetrachlorobis(tetrahydrofuran)titanium 31666-47-4 34946-82-2,
Copper(II) triflate 70317-90-7, Dichlorobis(tetrahydrofuran)iron
87863-62-5, Ytterbium tris(trifluoroacetate) 118821-99-1 139177-64-3,
Erbium triflate 179259-62-2 179259-63-3 179259-64-4 179259-65-5
179259-66-6 179259-67-7 179259-68-8 179259-69-9 179259-70-2
179259-71-3 179259-72-4 179259-73-5 179259-74-6 179259-75-7
179259-76-8 179259-77-9 179259-78-0

RL: CAT (Catalyst use); USES (Uses)

(hydrocyanation of pentenenitriles, alkylpentenoates, and
perfluoroalkylethenes with nickel(0) compds. and bidentate phosphorus
ligands as catalysts in presence of Lewis acid
promoters)

IT 179259-59-7P 179259-60-0P 179259-61-1P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)

(hydrocyanation of pentenenitriles, alkylpentenoates, and
perfluoroalkylethenes with nickel(0) compds. and bidentate phosphorus
ligands as catalysts in presence of Lewis acid
promoters)

IT 74-90-8, Hydrogen cyanide, reactions 591-80-0D, 4-Pentenoic
acid, esters, alkyl derivs. 592-51-8, 4-Pentenenitrile
602-09-5, [1,1'-Binaphthalene]-2,2'-diol 1079-66-9,
Chlorodiphenylphosphine 1806-29-7, 2,2'-Biphenol 4635-87-4,
3-Pentenenitrile 5204-64-8D, 3-Pentenoic acid, esters, alkyl derivs.
13284-42-9, 2-Pentenenitrile 13685-26-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrocyanation of pentenenitriles, alkylpentenoates, and
perfluoroalkylethenes with nickel(0) compds. and bidentate phosphorus
ligands as catalysts in presence of Lewis acid
promoters)

IT 111-69-3P, Adiponitrile 17611-82-4P, Ethylsuccinonitrile 28906-50-5P,
Methylglutaronitrile

RL: SPN (Synthetic preparation); PREP (Preparation)

(hydrocyanation of pentenenitriles, alkylpentenoates, and
perfluoroalkylethenes with nickel(0) compds. and bidentate phosphorus
ligands as catalysts in presence of Lewis acid
promoters)

IT 74-90-8, Hydrogen cyanide, reactions 592-51-8,
4-Pentenenitrile 4635-87-4, 3-Pentenenitrile 13284-42-9
, 2-Pentenenitrile

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrocyanation of pentenenitriles, alkylpentenoates, and
perfluoroalkylethenes with nickel(0) compds. and bidentate phosphorus
ligands as catalysts in presence of Lewis acid
promoters)

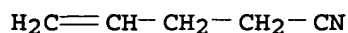
RN 74-90-8 HCAPLUS

CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)

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CH

RN 592-51-8 HCAPLUS

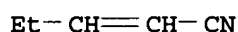
CN 4-Pentenenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 4635-87-4 HCAPLUS
 CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 13284-42-9 HCAPLUS
 CN 2-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L68 ANSWER 12 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1992:407528 HCAPLUS
 DN 117:7528
 TI **Hydrocyanation** of pentenenitriles using cyanohydrins
 IN Grunewald, Gerald C.
 PA du Pont de Nemours, E. I., and Co., USA
 SO U.S., 5 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 5107012	A	19920421	US 1991-691121	19910424
	JP 05112517	A2	19930507	JP 1992-99462	19920420
	JP 3205587	B2	20010904		
	CA 2066874	AA	19921025	CA 1992-2066874	19920422
	KR 226237	B1	19991015	KR 1992-6876	19920423
	EP 510689	A1	19921028	EP 1992-107057	19920424

R: BE, DE, ES, FR, GB, IT, NL

PRAI US 1991-691121 A 19910424

OS CASREACT 117:7528

AB **Hydrocyanation** of pentenenitriles using cyanohydrins as the HCN source and in which a solid dissociation additive is present in slurry to facilitate the dissociation of the cyanohydrin is described. Thus, **hydrocyanation** of a mixture of pentenenitriles (>98% of 3- and 4-pentenitrile) with acetone cyanhydrin in the presence of tetrakis(tritolyl phosphite)nickel, Ph3B and Al2O3 gave 92% adiponitrile.

IC ICM C07C253-30

INCL 558338000

CC 23-19 (Aliphatic Compounds)

ST **hydrocyanation** pentenenitrile cyanohydrin; adiponitrile

IT **Hydrocyanation**
 (of pentenenitriles)

IT **Hydrocyanation catalysts**
 (tetrakis(tritolyl phosphite)nickel, for pentenenitriles)

IT 71667-38-4

RL: CAT (Catalyst use); USES (Uses)

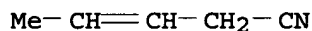
(catalyst, for **hydrocyanation** of pentenenitriles)

IT 75-86-5, Acetone cyanohydrin

RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrocyanation by, of pentenenitriles)
 IT 592-51-8, 4-Pentenenitrile 4635-87-4, 3-Pentenenitrile
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrocyanation of)
 IT 74-90-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrocyanation, of pentenenitriles)
 IT 111-69-3P, Adiponitrile
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 960-71-4, Triphenyl boron
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (promoter, for hydrocyanation of pentenenitriles)
 IT 592-51-8, 4-Pentenenitrile 4635-87-4, 3-Pentenenitrile
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrocyanation of)
 RN 592-51-8 HCAPLUS
 CN 4-Pentenenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 4635-87-4 HCAPLUS
 CN 3-Pentenenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 74-90-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrocyanation, of pentenenitriles)
 RN 74-90-8 HCAPLUS
 CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)



L68 ANSWER 13 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1991:163564 HCAPLUS
 DN 114:163564
 TI Preparation of adiponitrile
 IN Back, Gary L.; Batey, Harvey J.; Caton, John C.; Kump, Robin L.; O'Brien,
 Charles F., III; Robinson, Jacques D.
 PA du Pont de Nemours, E. I., and Co., USA
 SO U.S., 4 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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PI	US 4990645	A	19910205	US 1990-544625	19900627
	CA 2045721	AA	19911228	CA 1991-2045721	19910626

JP 04230254 A2 19920819 JP 1991-180552 19910626
 JP 2818503 B2 19981030
 EP 464691 A1 19920108 EP 1991-110691 19910627
 EP 464691 B1 19931215
 R: BE, DE, FR, GB, IT, NL
 KR 184879 B1 19990515 KR 1991-10751 19910627
 PRAI US 1990-544625 A 19900627
 AB Claimed is a process for the preparation of adiponitrile by the hydrocyanation of pentenenitrile using a zero-valent nickel catalyst and a triarylborane promoter in which solid catalyst degradation precipitate fouls the reactor and related equipment and is contained in the product fluid which comprises recycling a portion of the solid catalyst degradation precipitate to the reactor, and controlling the HCN concentration in the product stream leaving the reactor so that the HCN concentration does not exceed about 2500 ppm.
 IC ICM C07C253-10
 INCL 558335000
 CC 23-19 (Aliphatic Compounds)
 ST adiponitrile; pentenenitrile hydrocyanation
 IT Hydrocyanation
 (of pentenenitrile)
 IT 7440-02-0, Nickel, uses and miscellaneous
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst, in hydrocyanation of pentenenitrile)
 IT 592-51-8, 4-Pentenenitrile 27236-41-5, Pentenenitrile
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrocyanation of)
 IT 74-90-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrocyanation, of pentenenitrile)
 IT 111-69-3P, Adiponitrile
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, by hydrocyanation of pentenenitrile)
 IT 13283-31-3D, Borane, triaryl derivative
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (promoter, in hydrocyanation of pentenenitrile)
 IT 592-51-8, 4-Pentenenitrile
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrocyanation of)
 RN 592-51-8 HCAPLUS
 CN 4-Pentenenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 74-90-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (hydrocyanation, of pentenenitrile)
 RN 74-90-8 HCAPLUS
 CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)

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AN 1989:633036 HCAPLUS
DN 111:233036
TI Lewis acid effects on selectivity in nickel-catalyzed
pentenenitrile **hydrocyanation**. Triorganotin salts as tunable
Lewis acid **promoters**
AU McKinney, Ronald J.; Nugent, William A.
CS Cent. Res. Dev. Dep., E. I. du Pont de Nemours and Co., Wilmington, DE,
19880-0328, USA
SO Organometallics (1989), 8(12), 2871-5
CODEN: ORGND7; ISSN: 0276-7333
DT Journal
LA English
OS CASREACT 111:233036
AB Anhydrous triorganotin salts, R₃SnX (R = aryl, alkyl X = SbF₆, CF₃CO₂,
CF₃SO₃, MeC₆H₄SO₃) have been synthesized and utilized in exploring steric
and electronic effects on selectivity in nickel-catalyzed
pentenenitrile **hydrocyanation**. Steric effects dominate the
selectivity in the competition both between 3- and 4-pentenenitrile (3PN
and 4PN) **hydrocyanation** and between Markovnikov and
anti-Markovnikov addition of HCN to 4PN. Electronic effects, i.e., Lewis
acidity, effect only the activity of the **catalyst**, but in the
complex **hydrocyanation** system, this can result in yield changes
to adiponitrile.
CC 29-8 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 23
ST organotin salt effect **hydrocyanation** pentenenitrile; tin
triorgano salt prepn **promoter hydrocyanation**; steric
effect triorganotin **promoted hydrocyanation**;
electronic effect triorganotin **promoted hydrocyanation**
; regiochem **hydrocyanation** pentenenitrile Lewis acid effect
IT Inductive effect
Regiochemistry
Steric effect
(in nickel-catalyzed pentenenitrile **hydrocyanation**
promoted by triorganotin salts)
IT **Hydrocyanation**
(of pentenenitrile, nickel-catalyzed and triorganotin salt-
promoted)
IT Lewis acids
RL: RCT (Reactant); RACT (Reactant or reagent)
(triorganotin salts, effect of, on selectivity in nickel-
catalyzed pentenenitrile hydrocyanation)
IT 5162-44-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyanation of)
IT 29537-91-5 123835-26-7 123835-27-8 123835-28-9 123835-35-8
123835-36-9 123835-37-0
RL: PROC (Process)
(**hydrocyanation** of pentenenitrile in presence of)
IT 4635-87-4, 3-Pentenenitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrocyanation** of, nickel-catalyzed, effect of
triorganotin salts on selectivity in)
IT 74-90-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(**hydrocyanation**, of pentenenitrile, nickel-catalyzed
and triorganotin salt-**promoted**)
IT 1066-44-0, Trimethyltin bromide
RL: RCT (Reactant); RACT (Reactant or reagent)
(metathesis of, with silver hexafluoroantimonate)

- IT 2179-93-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(metathesis of, with triflic and trifluoroacetic acids)
- IT 2923-28-6, Silver trifluoromethanesulfonate
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation by, of triphenyltin hydride)
- IT 892-20-6, Triphenyltin hydride
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidation of, with silver trifluoromethanesulfonate)
- IT 20019-17-4P, Triphenyltin trifluoroacetate 27607-85-8P, Triphenyltin trifluoromethanesulfonate 90968-80-2P 90968-82-4P 90968-84-6P 123835-30-3P 123835-32-5P 123835-34-7P 123857-31-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and effect of, on selectivity and nickel-catalyzed pentenenitrile hydrocyanation)
- IT 25245-64-1P, Tri-tert-butyltin chloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and metathesis of, with silver hexafluoroantimonate)
- IT 592-51-8P, 4-Pentenitrile
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and nickel-catalyzed hydrocyanation of, effect of triorganotin salts on selectivity in)
- IT 19429-30-2P, Di-tert-Butyltin dichloride
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and tertiary-butylation of)
- IT 111-69-3P, Adiponitrile 4553-62-2P, 2-Methylglutaronitrile 17611-82-4P, Ethylsuccinonitrile
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, from hydrocyanation of pentenenitrile, nickel-catalyzed and triorganotin salt-promoted)
- IT 2767-54-6 7342-39-4 19464-54-1 60745-17-7 66952-23-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactions of)
- IT 677-22-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(tertiary-butylation by, of tin tetrachloride)
- IT 7646-78-8, Tin tetrachloride, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(tertiary-butylation of)
- IT 4635-87-4, 3-Pentenitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrocyanation of, nickel-catalyzed, effect of triorganotin salts on selectivity in)
- RN 4635-87-4 HCAPLUS
CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Me-CH=CH-CH₂-CN

- IT 74-90-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrocyanation, of pentenenitrile, nickel-catalyzed and triorganotin salt-promoted)
- RN 74-90-8 HCAPLUS
CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)

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IT 592-51-8P, 4-Pentenitrile
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and nickel-catalyzed hydrocyanation of,
effect of triorganotin salts on selectivity in)
RN 592-51-8 HCAPLUS
CN 4-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



L68 ANSWER 15 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1989:115486 HCAPLUS

DN 110:115486

TI Promoters for catalysts for hydrocyanation
of unsaturated nitriles

IN Hall, William T.; McKinney, Ronald J.; Nugent, William A.

PA du Pont de Nemours, E. I., and Co., USA

SO U.S., 5 pp.

CODEN: USXXAM

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4774353	A	19880927	US 1986-870895	19860605
PRAI	US 1986-870895		19860605		

OS CASREACT 110:115486; MARPAT 110:115486

AB The Ni(0)-catalyzed hydrocyanation of unsatd. nitriles
to dinitriles is promoted by the stannanes R₁R₂R₃SnX [R₁-R₃ =
alkyl, aryl (optionally substituted); X = non-nucleophilic anion of an
acid with pK_a <4]. Passing HCN gas into 10 mL of a 3-pentenitrile solution
of 2.94 g [(p-MeC₆H₄)₃PO]₄Ni and 2.50 mL (p-MeC₆H₄)₃P containing 1 equivalent
(based on Ni) Et₃SnSbF₆ stirred at 50-55° gave an 81.5% yield of
adiponitrile.

IC ICM C07C121-20

ICS C07C121-26

INCL 558335000

CC 35-2 (Chemistry of Synthetic High Polymers)

Section cross-reference(s): 23, 67

ST catalyst hydrocyanation nitrile unsatd; nickel compd
catalyst hydrocyanation; tin trialkyl catalyst
hydrocyanation; triethyltin fluoroantimonate catalyst
hydrocyanation; pentenenitrile hydrocyanation
catalyst; adiponitrile manuf catalyst

IT Hydrocyanation catalysts
(zero-valent nickel compds. and trialkyltin salts, for unsatd.
nitriles)

IT Nitriles, preparation

RL: IMF (Industrial manufacture); PREP (Preparation)

(di-, manufacture of, by hydrocyanation of unsatd. nitriles,
catalysts for)

IT Nitriles, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

- (unsatd., hydrocyanation of, catalysts for)
- IT 74-90-8, Hydrogen cyanide, uses and miscellaneous
RL: USES (Uses)
- (addition of, to unsatd. nitriles, catalysts for)
- IT 748-95-8, Tris(4-fluorophenyl)tintrifluoroacetate 1739-33-9,
Triphenyltintetrafluoroborate 3021-41-8, Triphenyltinsulfate (2:1)
4916-52-3 20019-17-4, Triphenyltintrifluoroacetate 27607-85-8,
Triphenyltintrifluoromethanesulfonate 29537-91-5 32261-35-1,
Tricyclohexyltintrifluoroacetate 36700-08-0 91312-01-5,
Triisopropyltintrifluoroacetate 103969-60-4,
Tribenzyltintrifluoroacetate 118821-82-2, Triethyltinhexafluoroantimonat
e 118821-83-3, Tripropyltinhexafluoroantimonate 118821-85-5,
Triisopropyltinhexafluoroantimonate 118821-86-6,
Triisopropyltintetrafluoroborate 118821-88-8,
Triisobutyltinhexafluoroantimonate 118821-90-2 118821-91-3,
Tri-t-butyltinhexafluoroantimonate 118821-93-5,
Trineopentyltinhexafluoroantimonate 118821-94-6,
Tricyclohexyltinhexafluoroantimonate 118821-96-8,
Tribenzyltinhexafluoroantimonate 118821-97-9,
Triphenyltinhexafluorophosphate 118821-98-0,
Triphenyltinhexafluoroantimonate 118821-99-1 118822-01-8,
Tris(4-fluorophenyl)tinhexafluoroantimonate 118858-57-4,
Tris[(trimethylsilyl)methyl]tinhexafluoroantimonate 119429-59-3,
Tris(2-methylphenyl)tintrifluoroacetate 119429-60-6,
Triisopropyltintrifluoromethanesulfonate 119429-61-7,
Trineopentyltintrifluoromethanesulfonate 119429-62-8,
Trineopentyltintrifluoroacetate 119429-63-9,
Tricyclohexyltintrifluoromethanesulfonate 119429-64-0,
Tricyclohexyltinperchlorate 119429-65-1 119588-40-8
RL: CAT (Catalyst use); USES (Uses)
- (catalysts, for hydrocyanation of unsatd. nitriles)
- IT 4635-87-4, 3-Pentenitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
- (hydrocyanation of, catalysts for)
- IT 111-69-3P, Adiponitrile
RL: IMF (Industrial manufacture); PREP (Preparation)
(manufacture of, by hydrocyanation of pentenenitrile,
catalysts for)
- IT 74-90-8, Hydrogen cyanide, uses and miscellaneous
RL: USES (Uses)
- (addition of, to unsatd. nitriles, catalysts for)
- RN 74-90-8 HCAPLUS
- CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)

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- IT 4635-87-4, 3-Pentenitrile
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrocyanation of, catalysts for)
- RN 4635-87-4 HCAPLUS
- CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Me-CH=CH-CH₂-CN

L68 ANSWER 16 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1988:416144 HCAPLUS

DN 109:16144

TI [Hexakis(pentenitrilo)nickel]bis- μ [(cyano)bis(triphenylborane) (I)],
its method of preparation and its use as a **promoter** for
hydrocyanation of pentenenitrile

IN Beatty, Richard Paul; Ostermaier, John Joseph

PA du Pont de Nemours, E. I., and Co., USA

SO Eur. Pat. Appl., 7 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 248643	A2	19871209	EP 1987-304884	19870603
	EP 248643	A3	19900207		
	EP 248643	B1	19930303		
	R: BE, DE, FR, GB, IT, LU, NL				
	US 4749801	A	19880607	US 1986-870739	19860604
	CA 1274245	A1	19900918	CA 1987-538225	19870528
	JP 62294691	A2	19871222	JP 1987-139074	19870604
	JP 08013832	B4	19960214		
PRAI	US 1986-870739	A	19860604		

AB [Ni(MeCH:CHCH₂CN)₆]²⁺ (Ph₃BCNBPh₃)₂²⁺ (I) is prepared as a **promoter**
for **hydrocyanation** of pentenenitrile to adiponitrile. Three
preparative methods are given, for example, 4.25 g
Ni[NC(CH₂)₄CN]₂[NCBPh₃]₂ was mixed with sufficient 3-pentenitrile to
give a slurry which was heated at .apprx.120° for 2 min, cooled,
and the filtrate was further cooled overnight to give I, which proved
comparable to Ph₃B as a **catalyst promoter** in the
hydrocyanation of 3-pentenitrile to adiponitrile. ORTEP
diagrams are given but no crystallog. is data presented.

IC ICM C07F015-04

ICS C07C120-02

CC 78-7 (Inorganic Chemicals and Reactions)

Section cross-reference(s): 35, 67

ST pentenenitrilenickel cyanophenyl borane complex **hydrocyanation**
promoter

IT Crystal structure

(of hexakis(pentenitrilo)nickel bis(μ -cyano)bis(triphenylborane))IT **Hydrocyanation**(of pentenenitrile, **promoters** for,
hexakis(pentenitrilo)nickel complexes as)

IT 13284-42-9, 2-Pentenitrile 17611-82-4, Ethylsuccinonitrile
28906-50-5, Methylglutaronitrile

RL: RCT (Reactant); RACT (Reactant or reagent)

(byproduct, from **hydrocyanation** of pentenenitrile, nickel
complex **promoter** for)

IT 36700-08-0

RL: CAT (Catalyst use); USES (Uses)

(catalyst, for **hydrocyanation** of pentenenitrile)

IT 4635-87-4, 3-Pentenitrile

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrocyanation of, adiponitrile from, nickel complex
promoter for)

IT 74-90-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(hydrocyanation, of pentenenitrile, **promoters** for,

hexakis(pentenitrilo)nickel complexes as)

IT 114715-69-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as **promoter** for **hydrocyanation** of
 penetenitrile)

IT 111-69-3P, Adiponitrile
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, via **hydrocyanation** of penetenitrile, nickel
 complex **promoter** for)

IT 87005-57-0
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with pentenenitrile, hexakis(pentenitrilo)nickel
 complex from)

IT 114822-05-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with triphenylborane, hexakis(penenitrilo)nickel
 complex from)

IT 13284-42-9, 2-Pentenitrile
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (byproduct, from **hydrocyanation** of penenenitrile, nickel
 complex **promoter** for)

RN 13284-42-9 HCAPLUS
 CN 2-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Et-CH=CH-CN

IT 4635-87-4, 3-Pentenitrile
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (**hydrocyanation** of, adiponitrile from, nickel complex
promoter for)

RN 4635-87-4 HCAPLUS
 CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

Me-CH=CH-CH₂-CN

IT 74-90-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (**hydrocyanation**, of penenenitrile, **promoters** for,
 hexakis(pentenitrilo)nickel complexes as)

RN 74-90-8 HCAPLUS
 CN Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)

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L68 ANSWER 17 OF 17 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1988:77623 HCAPLUS
 DN 108:77623
 TI Continuous **hydrocyanation** in dinitrile manufacture using zinc
 halide **promoter**
 IN Rapoport, Morris
 PA du Pont de Nemours, E. I., and Co., USA

SO U.S., 4 pp.
 CODEN: USXXAM
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 4705881	A	19871110	US 1986-930940	19861117
	CA 1297499	A1	19920317	CA 1987-551488	19871110
	JP 63135363	A2	19880607	JP 1987-285640	19871113
	JP 2521777	B2	19960807		
	EP 268448	A1	19880525	EP 1987-310107	19871116
	EP 268448	B1	19910918		
	R: BE, DE, FR, GB, IT, LU, NL				
PRAI	US 1986-930940	A	19861117		
AB	The continuous hydrocyanation of 3- and 4-pentenitrile by HCN to give adiponitrile is accomplished at 25-75° with Ni(0)-P(OR) ₃ complexes (R = aryl or substituted aryl containing ≤18 C) catalysts and with small amts. of ZnCl ₂ promoter , the feed stream having HCN/unsatd. nitrile molar ratio 0.35-0.8, the HCN/ catalyst molar ratio being 10-116, the HCN/ZnCl ₂ molar ratio being 30-800, and the ligand/Ni molar ratio being 5.4-8.2.				
IC	ICM C07C120-02				
INCL	558338000				
CC	45-4 (Industrial Organic Chemicals, Leather, Fats, and Waxes) Section cross-reference(s): 23				
ST	nickel hydrocyanation catalyst pentenenitrile; hydrogen cyanide continuous hydrocyanation pentenenitrile; zinc chloride hydrocyanation catalyst ; adiponitrile manuf hydrocyanation catalyst ; phosphite aryl complex hydrocyanation catalyst				
IT	Hydrocyanation catalysts (nickel complex-zinc chloride, for pentenenitrile to adiponitrile)				
IT	7440-02-0D, Nickel, complexes with tritolyl phosphite 7646-85-7, Zinc chloride, uses and miscellaneous 25586-42-9D, Tritolyl phosphite, complexes with Ni RL: CAT (Catalyst use); USES (Uses) (catalysts , for hydrocyanation of pentenenitrile)				
IT	74-90-8, Hydrogen cyanide, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (hydrocyanation by, of pentenenitrile, catalysts for)				
IT	592-51-8, 4-Pentenitrile 4635-87-4, 3-Pentenitrile RL: RCT (Reactant); RACT (Reactant or reagent) (hydrocyanation of, catalysts for)				
IT	111-69-3P RL: PREP (Preparation) (manufacture of, from pentenenitrile, hydrocyanation catalysts for)				
IT	74-90-8, Hydrogen cyanide, reactions RL: RCT (Reactant); RACT (Reactant or reagent) (hydrocyanation by, of pentenenitrile, catalysts for)				
RN	74-90-8 HCAPLUS				
CN	Hydrocyanic acid (8CI, 9CI) (CA INDEX NAME)				

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CH

IT 592-51-8, 4-Pentenitrile 4635-87-4, 3-Pentenitrile
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(hydrocyanation of, catalysts for)
RN 592-51-8 HCAPLUS
CN 4-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 4635-87-4 HCAPLUS
CN 3-Pentenitrile (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



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